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6. AUTHOR(S) RAJIV K. KALIA, AND PRIVA VASHISHTA			
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21 APR 1998

**FINAL TECHNICAL REPORT**

**AFOSR GRANT NUMBER: F49620-97-1-0265**

**PROGRAM MANAGER: Dr. ALEXANDER PECHENIK**

**COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE  
MATERIALS**

**PRINCIPAL INVESTIGATORS**

**RAJIV K. KALIA AND PRIYA VASHISHTA**

**Concurrent Computing Laboratory for Materials Simulations  
Department of Physics and Astronomy  
Department of Computer Science  
Louisiana State University, Baton Rouge, LA 70803-4001**

## **FINAL TECHNICAL REPORT (1997)**

**PROPOSAL TITLE:** COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS

**GRANT NUMBER:** F49620-97-1-0265

**PRINCIPAL INVESTIGATORS:** Rajiv K. Kalia and Priya Vashishta

**INSTITUTION:** Concurrent Computing Laboratory for  
Materials Simulations  
Department of Physics and Astronomy  
Department of Computer Science  
Louisiana State University  
Baton Rouge, LA 70803-4001  
Phone: (504) 388-1342  
Fax: (504) 388-5855  
Email: kalia@bit.csc.lsu.edu;

### **EXECUTIVE SUMMARY**

From July 30 - August 2, 1997 we organized an AFOSR supported international conference in Santa Fe, NM. The focus of the conference was on high-temperature materials with applications in defense technologies. The conference was attended by experimental and computational materials scientists, and experts in high performance computing and communications from universities, government laboratories, and industries in the U.S., Europe, and Japan. The topics covered at the meeting were: Synthesis, processing, and characterization of high-temperature materials; new algorithms and techniques for computer-aided design of materials; and virtual environments for materials design. The proceedings of the conference will be published by the Oxford University Press.

## TECHNICAL REPORT

The quest for high-temperature materials (HTMs) is one of the dominant themes in materials science and engineering. Novel materials that can withstand high temperatures and extreme environments are tremendously important for defense and civilian technologies. The basic requirements for designing materials that have low densities, elevated melting temperatures, high oxidation and corrosion resistance, the ability to resist creep, and high toughness encompass some of the most challenging problems in materials science. Despite a great deal of research focused on controlling structures at diverse length scales (atoms, defects, fibers, interfaces, grains, pores, etc.), many perplexing problems concerning mechanical properties and thermal behavior of HTMs as well as environmental effects at high temperatures remain unsolved.

An effective way of accelerating research in the area of HTMs is to have synergism between experiments, materials simulations, and high performance computing and communications (HPCC). In recent years we have witnessed rapid progress in large-scale atomistic simulations, highly efficient algorithms for massively parallel machines, and immersive and interactive virtual environments for analyzing and controlling simulations in real time. As a result of these advances, simulations can now reliably predict properties of materials in advance of fabrication. Thus, materials simulations are capable of complementing and guiding the experimental search for novel HTMs.

To accelerate the pace of experimental research on HTMs through synergism with computational efforts, we received a grant from the Air Force Office of Scientific Research to organize an international conference called "Computer-Aided Design of High-Temperature Materials." The conference was held from July 30 - August 2, 1997 in Santa Fe, NM. The meeting brought together experimental and computational materials scientists and engineers with expertise in atomistic and continuum approaches and grand challenge applications. The conference provided experimental and computational materials scientists/engineers with a forum to exchange ideas and discuss the latest developments in HTMs. The meeting focused on the following topics:

- High-temperature ceramics, composites, intermetallic compounds, and nanophase materials;
- Phase stability, thermal stability, oxidation resistance, and thermal shock resistance of HTMs;

- Measurements and modeling of residual stresses, growth of defects, effects of high strain and strain rates, creep behavior, fracture, and the effect of environment on HTMs;
- *Ab initio* electronic structure, molecular dynamics, Monte Carlo, and continuum approaches for high-temperature material simulations;
- Parallel algorithms for materials simulations and immersive and interactive visualization environments for virtual design of materials.

The proceedings, featuring papers presented at the conference, will be published by the Oxford University Press.

As a supplement to this technical report, we are attaching the following documents:

- Material for conference announcement including the poster;
- Abstract book which includes the conference program.

# CAD/HTM

## Computer-Aided Design of High-Temperature Materials

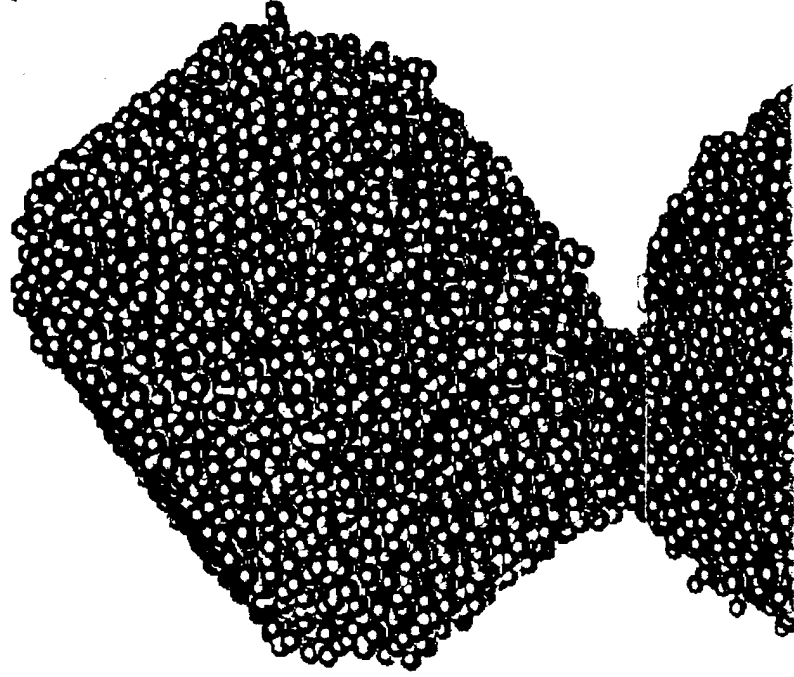
**Santa Fe, New Mexico  
July 30– Aug 2, 1997**

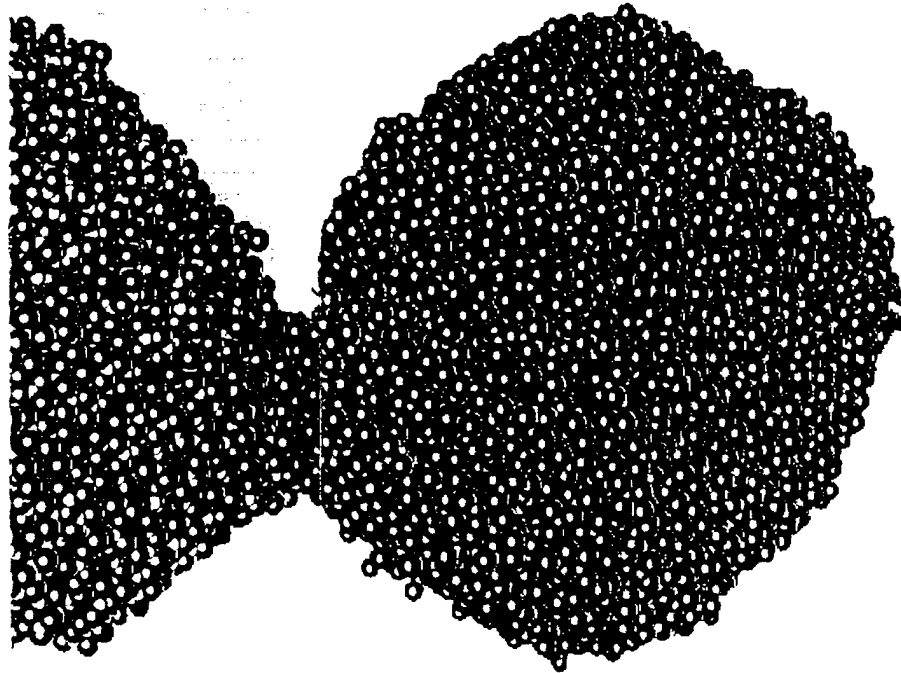
### Call for Papers

Abstracts are invited for oral and poster presentations.  
Please submit an abstract (250 words maximum) via  
E-mail, mail, or fax. Abstract deadline: July 1, 1997.  
Send abstracts to:

Ms. Arnell Jackson  
Department of Physics and Astronomy  
Louisiana State University  
Baton Rouge, LA 70803-4001  
Phone: (504) 388-1342  
Fax: (504) 388-5855  
E-mail: [htm@rouge.phys.lsu.edu](mailto:htm@rouge.phys.lsu.edu)

### Conference Organizers





②

## **The Aim**

The purpose of this conference is to provide experimental and computational scientists with a forum to exchange ideas and discuss the latest developments in high-temperature materials (HTMs). The goal is to identify the areas of research in HTMs that can benefit the most from collaborations between experimental and computational materials scientists. The emphasis of this conference is on establishing strong lines of communication and theme building. The conference will feature presentations on state-of-the-art materials modeling and recent experimental developments in HTMs.

## **The Topics**

Please submit an abstract (250 words maximum) via E-mail, mail, or fax. Abstract deadline: July 1, 1997. Send abstracts to:

Ms. Arnell Jackson  
Department of Physics and Astronomy  
Louisiana State University  
Baton Rouge, LA 70803-4001  
Phone: (504) 388-1342  
Fax: (504) 388-5855  
E-mail: htm@rouge.phys.lsu.edu

## **Conference Organizers**

Rajiv K. Kalia and Priya Vashishta  
Louisiana State University

Alexander Pechenik  
Air Force Office of Scientific Research

## **Registration**

The registration fee of \$275 (\$250 before July 1, 1997) per person includes all conference sessions, breaks, lunch, and refreshments (Wed., Thurs., Fri., & Sat.). For more information about registration, please contact LSU Conference Services and return the enclosed card.

Phone: (504) 388-6264 or 1 (800) 256-6948  
Fax: (504) 388-6324.

## **Location**

Doubletree Hotel,  
3347 Cerillos Road  
Santa Fe, New Mexico 87505  
Phone: (505) 473-2800, 1 (800) 777-3347  
Fax: (505) 473-5128  
Please make reservations by July 1, 1997

## **For Information**

For more information about registration or lodging, please contact:

Linda W. Lightfoot, Conference Coordinator

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## The Topics

Fundamentals of HTM phenomena and properties of ceramics, composites, intermetallic compounds, and other high-temperature structural materials.

Measurements and modeling of interfacial phenomena, stresses, growth of defects, effects of high strain and strain rates, creep behavior, and fracture in HTMs.

Electronic structure, molecular dynamics, Monte Carlo, and continuum approaches as applied to the complete description and prediction of HTM properties.

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Please make reservations by July 1, 1997

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LSU Conference Services  
(504) 388-6264 or 1 (800) 256-6948  
FAX: (504) 388-6324  
E-mail: llightfoot@lanmail.ocs.lsu.edu.

For Program Information, contact:

Rajiv K. Kalia or Priya Vashishta  
**Concurrent Computing Laboratory for  
Materials Simulations**

Department of Physics and Astronomy  
Department of Computer Science  
Nicholson Hall  
Louisiana State University  
Baton Rouge, Louisiana 70803-4001  
Phone (504) 388-1342; Fax: (504) 388-5855  
E-mail: htm@rouge.phys.lsu.edu

To receive more information, please return the enclosed card.

## Partial List of Invited Speakers

Alan J. Ardell (UCLA)

*Coarsening of Eutectic and Discontinuous Lamellar Microstructures*

Elisabeth Bouchaud (O.N.E.R.A., France)

*Scaling Properties of Cracks*

Jeremy Broughton (NRL)

*Integrating Electronic, Atomistic and Continuum Length Scales in Simulations*

Long-Qing Chen (Penn State)

*Modeling Microstructural Evolution Under Externally Applied Stresses*

Donald Ellis (Northwestern)

*Hybrid Classical and Quantum Modelling of Defects, Interfaces, and Surfaces*

Andreas M. Glaeser (Berkeley)

*Fundamental Studies of Surfaces and Interfaces at High Temperature via*

*Microdesigned Interfaces*

*Electric Gradients (Continued)*

Peter E. D. Morgan (Rockwell)

*Chemical Methods for Processing La-Monazite and Related Compounds for CMC Weak Interfaces*

David G. Pettifor (Oxford)

*Bond-Order Potentials: Bridging the Electronic-Atomistic Length Scale Gap for High Temperature Covalent Ceramics and Intermetallics*

Rishi Raj (Colorado)

*Simulations of Variability in High Temperature Mechanical Properties Emanating from Statistically Distributed Microstructural Parameters of Ceramics*

Michael D. Sacks (Florida)

*High-Temperature Silicon Carbide Fibers*

Ali Sayir (NASA)

*Directional Solidification of Ceramic Eutectics*

John Smith (General Motors)

*Electrochemical Effects in Solid Oxide Fuel Cells*



Electronic structure, molecular dynamics, Monte Carlo, and continuum approaches as applied to the complete description and prediction of HTM properties.

## Materials Simulations

Department of Physics and Astronomy  
Department of Computer Science  
Nicholson Hall  
Louisiana State University  
Baton Rouge, Louisiana 70803-4001  
Phone (504) 388-1342; Fax: (504) 388-5855  
E-mail: htm@rouge.phys.lsu.edu

To receive more information, please return the enclosed card.

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**Andreas M. Glaeser (Berkeley)**

*Fundamental Studies of Surfaces and Interfaces at High Temperature via Microdesigned Interfaces*

**Leslie Greengard (Courant)**

*Elastostatics of Composite Materials*

**Martin P. Harmer (Lehigh)**

*Grain Boundary Chemistry and Creep Resistance of Alumina*

**Armen G. Khachatryan (Rutgers)**

*Computer Simulation of Microstructure in Metal and Ceramic Systems. Near or Remote Future*

**Masanori Kohyama (ONRI, Japan)**

*Ab Initio Calculations of Interfaces in Materials: Grain Boundaries in SiC and SiC-Al Interfaces*



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**Peter E. D. Morgan (Rockwell)**

*Chemical Methods for Processing La-Monazite and Related Compounds for CMC Weak Interfaces*

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**John Smith (General Motors)**

*Universal Behavior in Adhesion of Some High Temperature Materials*

**Rick Stevens (Argonne)**

*Collaborative and Virtual Environments to Support Large Scale Computational Science*

**Kiyoyuki Terakura (JRCAT, Japan)**

*Atomic and Molecular Processes on Si and in Zeolites Studied by First-Principles Molecular Dynamics*

**Vasek Vittek (Penn)**

*Mechanism of Cooperative Generation of Dislocations and Brittle-to-Ductile Transition*

**Renata Wentzcovitch (Minnesota)**

*Polymorphs of Alumina Predicted by First Principles: Putting Pressure on the Ruby Pressure Scale*

**Sidney Yip (MIT)**

*Atomic-Level Mechanisms of Interfacial Deformation*

# 1997

## CONFERENCE ON COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS

July 30 - August 2, 1997

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April 28, 1997

RE: Conference on Computer-Aided Design of High-Temperature Materials

July 30 - August 2, 1997 Santa Fe, New Mexico

e-mail: [htm@rouge.phys.lsu.edu](mailto:htm@rouge.phys.lsu.edu)

URL: <http://www.cclms.lsu.edu/>

Dear Colleague:

We would like to invite you to participate in a conference on fundamental phenomena in high-temperature materials (HTMs), which is being sponsored by the Air Force Office of Scientific Research.

The purpose of this conference is to provide experimental and computational scientists with a forum to exchange ideas and discuss the latest developments in HTMs. The goal is to identify the areas of research in HTMs that can benefit the most from collaborations between experimental and computational materials scientists. The emphasis of this conference is on establishing strong lines of communication and theme building. The conference will feature presentations on state-of-the-art materials modeling and recent experimental developments in HTMs.

The conference will focus on the following topics:

- Fundamentals of HTM phenomena and properties of ceramics, composites, intermetallic compounds, and other high-temperature structural materials;
- Measurements and modeling of interfacial phenomena, stresses, growth of defects, effects of high strain and strain rates, creep behavior, and fracture in HTMs;
- Electronic structure, molecular dynamics, Monte Carlo, and continuum approaches as applied to the complete description and prediction of HTM properties.

The conference format will consist of morning and afternoon sessions featuring invited and contributed talks and a poster session. The proceedings of the conference will be published by the Oxford University Press.

Enclosed you will find the conference poster and registration form. If you have any questions, please do not hesitate to contact us.

Yours sincerely,



Lindsey Lightfoot

LSU Conference Services

177 Pleasant Hall

Baton Rouge, LA 70803-1520

Ph: 504-388-6264; Fax: 504-388-6324

[llightfoot@lanmail.ocs.lsu.edu](mailto:llightfoot@lanmail.ocs.lsu.edu)

# 1997

## CONFERENCE ON COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS

July 30 - August 2, 1997

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### Registration

The registration fee of \$275 (\$250 before July 1, 1997) per person entitles registrants to all conference sessions and breaks. Registration also includes the Welcome reception on Tuesday, and lunch on Wednesday, Thursday, Friday, Saturday. Drinks and refreshments will be served on Wednesday, Thursday, and Friday evenings. To register, please complete the enclosed registration form and mail it with a check to:

LSU Conference Services  
177 Pleasant Hall  
Louisiana State University  
Baton Rouge, LA 70803-1503

You may register by phone or fax, using Visa, MasterCard or American Express. Please include a completed registration form or facsimile with your registration.

**Phone:** 504-388-6264 or 1-800-256-6948  
**FAX:** 504-388-6324

### Accommodations

All conference sessions will be held at the Doubletree Hotel, Santa Fe. A block of rooms is available to conference participants at a special conference rate of \$109 for standard rooms, \$129 for suites. Breakfast is included in this rate. **Please make your reservations directly with the hotel by July 1, 1997 and mention the group name CERAM to receive this special rate.**

Doubletree Hotel of Santa Fe  
3347 Cerillos Road  
Santa Fe, New Mexico 87505  
**Phone:** 505-473-2800; 1-800-777-3347  
**FAX:** 505-473-5128

This room block will be released July 1, so we encourage you to make your reservations as early as possible.

### Transportation

**CAR RENTAL:** Avis is the official car rental agency for the conference. The Avis Worldwide Discount (AWD) number is A6098499. Please use this number when making reservations in order to receive special discounted rates. Reservations may be made by calling the Meeting Reservation and Information Desk at 1-800-331-1600.

**FLIGHT INFORMATION:** Delta Air Lines is the official air carrier and Louisiana Travel is the official travel agency for the conference. Delta is offering special discounted meeting fares. Please make all airline reservations by calling Louisiana Travel at 1-888-930-6700. Please mention the Computer-Aided Design Conference and give the file number 101374A.

**SHUTTLES:** The Albuquerque airport is approximately one hour from Santa Fe. Shuttle Jack provides shuttle service from the airport to Santa Fe. Buses depart from the terminal in front of Southwest Airlines at the ground level. The cost of a one-way ticket is \$20. If you would like to pay with Visa or MasterCard, you must make your reservation in advance by calling 505-243-3244. A Shuttle Jack schedule will be sent with your registration confirmation.

### Opera

The 1997 opera season runs from June 27-August 23. Contact the Santa Fe Opera at 1-800-280-4654 for ticket information.

### For More Information

For more information about registration or lodging, please contact:

Lindsey Lightfoot, Conference Coordinator  
LSU Conference Services  
504-388-6264 or 1-800-256-6948  
**FAX:** 504-388-6324  
E-mail: [llightfoot@lanmail.ocs.lsu.edu](mailto:llightfoot@lanmail.ocs.lsu.edu)

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Department of Physics and Astronomy  
Department of Computer Science  
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**FAX:** 504-388-5855  
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*Announcing*

## Computer-Aided Design of High-Temperature Materials

Edited by Alexander Pechenik, Rajiv K. Kalia, and Priya Vashishta

High-temperature materials is a fast-moving research area with numerous practical applications. Materials that can withstand extremely high temperatures and extreme environments are generating considerable attention worldwide; however, designing materials that have low densities, elevated melting temperatures, oxidation resistance, creep resistance, and intrinsic toughness encompass some of the most challenging problems in materials science.

The current search for high-temperature materials is largely based on traditional, trial-and-error experimental methods which are costly and time-consuming. An effective way to accelerate research in this field is to use recent advances in materials simulations and high performance computing and communications (HPCC) to guide experiments. This synergy between experiment and advanced materials modeling will significantly enhance the synthesis of novel high-temperature materials.

This volume will collect the proceedings from the **International Conference on Computer-Aided Design of High-Temperature Materials**, which will take place July 30-August 2, 1997. The conference will be a forum for experimental and computational scientists to discuss current work in high-temperature materials and will emphasize the potential for collaboration. It will feature state-of-the-art materials modeling and recent experimental developments in high-temperature materials. The conference will focus on the following topics:

- Fundamentals of high-temperature material (HTM) phenomena and properties of ceramics, composites, intermetallic compounds, and other high-temperature structural materials;
- Measurements and modeling of interfacial phenomena, stresses, growth of defects, effects of high strain and strain rates, creep behavior, and fracture in HTM's;
- Electronic structure, molecular dynamics, Monte Carlo and continuum approaches as applied to the complete description of HTM properties.

The proceedings will be published in March 1998 and the tentative price is \$75.00

About the Editors:

**Alexander Pechenik** is Program Manager at the Air Force Office of Scientific Research.

**Rajiv K. Kalia** is Professor of Physics and Computer Science at Louisiana State University.

**Priya Vashishta** is Cray Research Professor of Computational Science and Professor of Physics and Computer Science at Louisiana State University.

*See reverse for ordering information.*

**For ordering information, contact**

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*The Doubletree Hotel-Santa Fe would like to welcome  
all attendees of the*

# 1997

## CONFERENCE ON COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS

**JULY 30 - AUGUST 2, 1997**

As host hotel for the upcoming **Computer-Aided Design of High-Temperature Materials Conference**, we would like to extend our warmest welcome to all attending. The group code for your room block is "**CERAM**." Your group rate is \$109 per night, which is taxed at 10.25%, for an inclusive total of \$120.18 per night. This rate includes a daily breakfast buffet in our restaurant.

Please fax this sheet to us at 505-473-5128 or email your reservation request to dtreesf@rt66.com. We will be happy to fax or email confirmation; please let us know your preference.

---

NAME \_\_\_\_\_

ADDRESS \_\_\_\_\_

PHONE \_\_\_\_\_ FAX \_\_\_\_\_

EMAIL ADDRESS \_\_\_\_\_

GROUP CODE: **CERAM**

RATE: **\$109 (INCLUDES BREAKFAST)**

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☐ SMOKING

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**3347 CERRILLOS ROAD**  
**SANTA FE, NM 87505**

**Reservations: 1-800-777-3347**

**Phone: 505-473-2800**

**Fax: 505-473-5128**

**Email: dtreesf@rt66.com**

# 1997 CONFERENCE ON COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS

**JULY 30 - AUGUST 2, 1997**

The registration fee of **\$275** (\$250 before July 1, 1997) per person entitles registrants to all conference sessions and breaks. Registration also includes the Welcome Reception on Tuesday, and lunch on Wednesday, Thursday, Friday, and Saturday. Drinks and refreshments will be served on Wednesday, Thursday, and Friday evenings. To register, please complete the enclosed registration form and mail it with a check to:

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Baton Rouge, LA 70803-1503

You may also register by phone or fax, using Visa, MasterCard or American Express. Please include a completed registration form or facsimile with your registration.

**Phone:** 504-388-6264 or 1-800-256-6948

**FAX:** 504-388-6324

FOR MORE INFORMATION about registration, please contact Lindsey Lightfoot, Conference Coordinator, at LSU Conference Services: 504-388-6264; Fax: 504-388-6324

REFUND POLICY: A 90% refund will be given if written notice or a faxed letter of cancellation is received in the Short Courses office no later than July 18, 1997.

## CONFERENCE REGISTRATION FORM

Louisiana State University  
Short Courses and Conferences  
177 Pleasant Hall  
Baton Rouge, LA 70803  
504-388-6264 · 800-256-6948 · Fax: 504-388-6324

### PARTICIPANT INFORMATION

NAME \_\_\_\_\_

INSTITUTION \_\_\_\_\_

ADDRESS \_\_\_\_\_

CITY \_\_\_\_\_ STATE \_\_\_\_\_ ZIP \_\_\_\_\_

PHONE \_\_\_\_\_ FAX \_\_\_\_\_

EMAIL \_\_\_\_\_ SSN# \_\_\_\_\_

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☐ I HAVE SENT MY HOTEL REGISTRATION FORM TO THE DOUBLETREE HOTEL.

### COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS (FHTMC81)

**JULY 30 - AUGUST 2, 1997**

**EARLY FEE (BEFORE JULY 1, 1997): \$250**

**FEE AFTER JULY 1, 1997: \$275**

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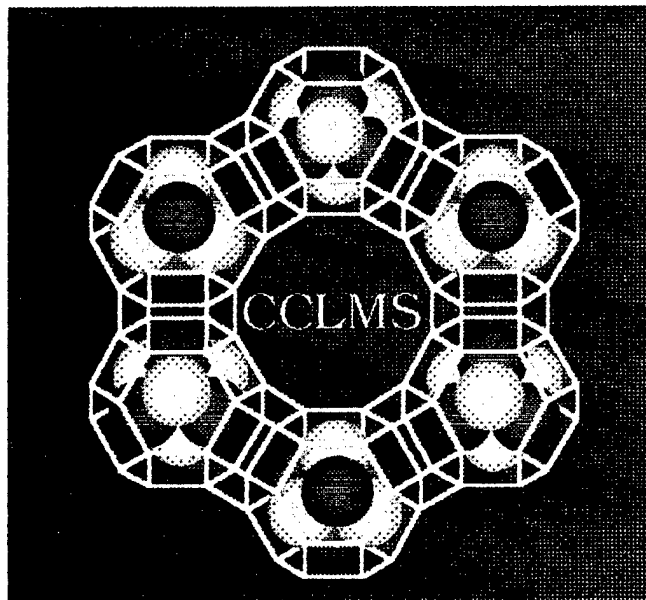
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**CONCURRENT COMPUTING LABORATORY  
FOR MATERIALS SIMULATIONS**

**Computer-Aided Design of  
High-Temperature Materials**  
Conference Program & Abstracts

Supported by  
**Air Force Office of Scientific Research**

Santa Fe, New Mexico  
**July 30 - August 2, 1997**



**DTIC QUALITY INSPECTED 3**

DEPARTMENT OF PHYSICS AND ASTRONOMY  
AND  
DEPARTMENT OF COMPUTER SCIENCE  
**LOUISIANA STATE UNIVERSITY**



# **Computer-Aided Design of High-Temperature Materials Conference Program & Abstracts**

**Doubletree Hotel  
Santa Fe, New Mexico  
July 30 - August 2, 1997**

## **Organizers**

**Alexander Pechenik  
Air Force Office of Scientific Research  
and  
Rajiv K. Kalia & Priya Vashishta  
Louisiana State University**

**DTIC QUALITY INSPECTED 2**

**Supported by  
Air Force Office of Scientific Research**

**COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS**  
**SANTA FE, NM, JULY 30 - AUGUST 2, 1997**  
**TENTATIVE AGENDA FOR THE CONFERENCE**

**WEDNESDAY MORNING, JULY 30**

**Alexander Pechenik (AFOSR)** 8:00 - 8:25 AM  
Opening Remarks

**Chairperson: Alexander Pechenik (AFOSR)**

**Bruce Taggart (NSF)** 8:25 - 8:50 AM  
NSF Programs on Computer Aided Design of High Temperature Materials

**Sheldon Wiederhorn (NIST)** 8:50 - 9:25 AM  
Creep Deformation of Silicon Nitride

**Rishi Raj (Colorado)** 9:25 - 10:00 AM  
Simulations of Variability in High Temperature Mechanical Properties  
Emanating from Statistically Distributed Microstructural Parameters of Ceramics

**COFFEE** 10:00 - 10:30 AM

**Chairperson: Alexander Pechenik (AFOSR)**

**Martin Harmer (Lehigh)** 10:30 - 11:05 AM  
Grain Boundary Chemistry and Creep Resistance of Alumina

**Renata Wentzcovitch (Minnesota)** 11:05 - 11:40 AM  
Polymorphs of Alumina Predicted by First Principles: Putting Pressure  
on the Ruby Pressure Scale

**David Price (Argonne)** 11:40 - 12:15 PM  
Structure and Transport in Levitated Melts

**Richard A. Page (Southwest Research Institute)** 12:15 - 12:30 PM  
Creep Damage Processes in Structural Ceramics: Experimental Studies  
and Their Implications for Computational Modeling

**LUNCH** 12:30 - 2:00 PM

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**WEDNESDAY AFTERNOON, JULY 30**

**Chairperson:** Joanna McKittrick (Univ. of California at San Diego)

**Michael Sacks (Univ. of Florida)** 2:00 - 2:35 PM  
High-Temperature Silicon Carbide Fibers

**Sidney Yip (MIT)** 2:35 - 3:10 PM  
Insights on Deformation Mechanisms from Atomistic Modeling of  
Structural Instability in Solids

**P. C. Clapp (Univ. of Connecticut)** 3:10 - 3:25 PM  
SiC: Growth, Sintering & Thermal Conductivity

**COFFEE** 3:25 - 3:50 PM

**Chairperson: Jeffrey Rickman (Lehigh)**

**Andrey Omeltchenko (Louisiana State Univ.)** 3:50 - 4:25 PM  
Dynamic Fracture in Nanophase Ceramics and Diamond Films:  
Multimillion Atom Parallel Molecular-Dynamics Simulations

**Elisabeth Bouchaud (O.N.E.R.A., France)** 4:25 - 5:00 PM  
Scaling Properties of Cracks

<b>P. Peralta (Los Alamos)</b>	5:00 - 5:15 PM
Effect of Small Aluminum Additions on Mechanical, Elastic and Structural Properties of Monocrystalline C11b MoSi <sub>2</sub>	

**S. P. Chen (Los Alamos)** 5:15 - 5:30 PM  
A Total Energy Study of Phase Stability and Mechanical Properties  
of Laves Phase Compounds

**REFRESHMENTS** 6:00 - 7:30 PM

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**SANTA FE, NM, JULY 30 - AUGUST 2, 1997**  
**TENTATIVE AGENDA FOR THE CONFERENCE**

**THURSDAY MORNING, JULY 31**

**Chairperson:** Arje Nachman (AFOSR)

**Anna Tsao (DARPA)** 8:00 - 8:25 AM

<b>Leslie Greengard (Courant)</b> Nearly Singular Fields: Electrostatics and Elastostatics of Composite Materials	8:25 - 9:00 AM
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**Kaushik Bhattacharya (Caltech)** 9:00 - 9:35 AM  
 Energy-Based Model of Compressive Splitting in Heterogeneous Brittle Solids

<b>Oscar Bruno (Caltech)</b> Microscopic Misfit Strains in Polycrystals	9:35 - 10:10 AM
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**COFFEE** 10:10 - 10:40 AM

**Chairperson:** William Petuskey (Arizona State Univ.)

<b>Alan Ardell (UCLA)</b> Coarsening of Eutectic and Discontinuous Lamellar Microstructures	10:40 - 11:15 AM
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<p><b>Armen Khachaturyan (Rutgers)</b>          Computer Simulation of Microstructure in Metal and Ceramic Systems.          Near or Remote Future</p>	<p>11:15 - 11:50 AM</p>
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**Robin Selinger (Catholic Univ.)** 11:50 - 12:05 PM  
**Fingering Instability in Dislocation Annihilation**

**Veena Tikare (Sandia)** 12:05 - 12:20 PM  
Monte Carlo Simulation of Ostwald Ripening

**Dipanwita Banerjee (Ohio State)** 12:20 - 12:35 PM  
 Continuum Field Kinetic Model and Simulation of Precipitation of L12  
 Ordered Intermetallics from fcc Solid Solution

**LUNCH** 12:35 - 2:00 PM

**COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS**  
**SANTA FE, NM, JULY 30 - AUGUST 2, 1997**  
**TENTATIVE AGENDA FOR THE CONFERENCE**

**THURSDAY AFTERNOON, JULY 31**

**Chairperson:** Jenn-Ming Yang (UCLA)

**Ali Sayir (NASA)** 2:00 - 2:35 PM  
Directional Solidification of Eutectic Ceramics

**Long-Qing Chen (Penn State)** 2:35 - 3:10 PM  
Modeling Microstructural Evolution Under Externally Applied Stresses

**Danan Fan (Los Alamos)** 3:10 - 3:25 PM  
Computer Simulation of Grain Growth Kinetics with Solute-Drag Using  
Phase Field Model

**COFFEE** 3:25 - 3:50 PM

**Chairperson: David Marshall (Rockwell)**

**Peter E. D. Morgan (Rockwell)** 3:50 - 4:25 PM  
The Interface Between Monazites and High Temperature Ceramics

**John Smith (General Motors)** 4:25 - 5:00 PM  
Universal Behavior in Adhesion of Some High Temperature Materials

<b>Martina Bachlechner (Louisiana State Univ.)</b> Structural Correlations and Stress Distributions at Silicon/Silicon Nitride Interface	5:00 - 5:15 PM
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**C.-K. Loong (Argonne)** 5:15 - 5:30 PM  
The Processing and Functionality of Nitride, Oxide, and Phosphate  
Ceramics Characterized by Neutron Scattering

**J. W. Richardson, Jr. (Argonne)** 5:30 - 5:45 PM  
Neutron Scattering Characterization of Microstructure in Uranium Silicides,  
Ceramic Composites and Ni-based Alloys

**REFRESHMENTS** 6:00 - 7:30 PM

**COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS**  
**SANTA FE, NM, JULY 30 - AUGUST 2, 1997**  
**TENTATIVE AGENDA FOR THE CONFERENCE**

**FRIDAY MORNING, AUGUST 1**

**Chairperson:** Carl Kukkonen (JPL)

<b>Andreas Glaeser (Berkeley)</b> Fundamental Studies of Surfaces and Interfaces at High Temperature via Microdesigned Interfaces	8:00 - 8:35 AM
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**David Pettifor (Oxford)** 8:35 - 9:10 AM  
 Bond-Order Potentials: Bridging the Electronic-Atomistic Length Scale Gap  
 for High Temperature Covalent Ceramics and Intermetallics

**Masanori Kohyama (ONRI, Japan)** 9:10 - 9:45 AM  
Ab Initio Calculations of Interfaces in Materials: Grain Boundaries in SiC and SiC-Al Interfaces

**Kenji Tsuruta (Louisiana State Univ.)** 9:45 - 10:00 AM  
 Structure and Dynamics of Consolidation and Fracture of Nanophase  
 Ceramics via Parallel Molecular Dynamics

**COFFEE** 10:00 - 10:30 AM

**Chairperson:** John Mundy (DOE)

**Richard Goettler (Babcock & Wilcox)** 10:30 - 11:05 AM  
Interfaces in Oxide Fiber-Oxide Matrix Ceramic Composites

**Donald Ellis (Northwestern Univ.)** 11:05 - 11:40 AM  
Hybrid Classical and Quantum Modelling of Defects, Interfaces, and Surfaces

**Lin Yang (Livermore)** 11:40 - 11:55 AM  
 Structural Properties of SiO<sub>2</sub> under Pressures: First-principles Calculations  
 and Database for Several Crystalline Configurations

**José P. Rino (São Carlos, Brasil)** 11:55 - 12:10 PM  
Structural Correlations of Amorphous Silica at High Pressures

**H. Iyetomi (Niigata Univ., Japan)** 12:10 - 12:25 PM  
 Development of a Variational APW Method and its Application to  
 the Electronic Properties of Ionic compounds

**H. Kikuchi (Niigata Univ., Japan)** 12: 25 - 12:40 PM  
Band-theoretical Approach to the Superionic Conductivity of Solid Electrolytes

**LUNCH** 12:40 - 2:00 PM

**COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS**  
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**TENTATIVE AGENDA FOR THE CONFERENCE**

**FRIDAY AFTERNOON, AUGUST 1**

**Chairperson:** Sheldon Wiederhorn (NIST)

**Ronald Kerans (Wright Lab)** 2:00 - 2:35 PM  
Research Challenges in the Development of Ceramic Composites

**Christopher Woodward (UES Inc.)** 2:35 - 3:10 PM  
Computational Material Science as a Tool for Alloy Development:  
Understanding the Influence of Chemistry on Flow Behavior in TiAl

**J. J. Mecholsky (Univ. of Florida)** 3:10 - 3:25 PM  
Quantum Mechanics, Fracture Mechanics and Fractal Geometry  
Applied to High Temperature Materials

**COFFEE** 3:25 - 3:50 PM

**Chairperson:** Charles Holland (AFOSR)

**Christian Mailhot (Livermore)** 3:50 - 4:25 PM  
Multiscale Materials Modeling at LLNL: Plastic Flow in bcc Metals

<b>Rick Stevens (Argonne)</b> Collaborative and Virtual Environments to Support Large Scale Computational Science	4:25 - 5:00 PM
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**Aiichiro Nakano (Louisiana State Univ.)** 5:00 - 5:15 PM  
**Multilevel Algorithms for Computational High-Temperature Materials Research**

**M. L. Wang (Univ. of Illinois, Chicago)** 5:15 - 5:30 PM  
Modified Gauss Points Methods and its Application in HTMs

**Bruce R. Patton (Ohio State Univ.)** 5:30 - 5:45 PM  
**Simulating High Temperature Ceramic Sensors Across All Length Scales**

**REFRESHMENTS** 6:00 - 7:30 PM

**COMPUTER-AIDED DESIGN OF HIGH-TEMPERATURE MATERIALS**  
**SANTA FE, NM, JULY 30 - AUGUST 2, 1997**  
**TENTATIVE AGENDA FOR THE CONFERENCE**

**SATURDAY MORNING, AUGUST 2**

**Chairperson:**        **Jack Mecholsky (Univ. of Florida)**

<b>Hamish Fraser (Ohio State)</b>	8:00 - 8:35 AM
Issues Involving Ductility, Toughness, and Structural Stabilities in Intermetallics and Multilayered High Temperature Materials	

<b>Peter Lomdahl (Los Alamos)</b>	8:35 - 9:10 AM
Large Scale Parallel Molecular Dynamics Simulations of Ductile Failure	

<b>Donald Brenner (NC State)</b>	9:10 - 9:45 AM
Multiscale Modeling Method for Predicting Mechanical Properties of Polycrystalline Covalent Ceramics from First Principles	

<b>Kai Wang (NC State)</b>	9:45 - 10:00 AM
High Temperature Thermal Property Predictions for MgO, KCl and ZnS	

<b>P. Zeng (Univ. of Connecticut)</b>	10:00 - 10:15 AM
Tests of Sintering Laws at the Nanoscale	

<b>COFFEE</b>	10:15 - 10:45 AM
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**Chairperson:**        **Shuji Ogata (Yamaguchi Univ., Japan)**

<b>Kiyoyuki Terakura (JRCAT, Japan)</b>	10:45 - 11:20 AM
Atomic and Molecular Processes Studied by First-Principles Molecular Dynamics	

<b>Jeremy Broughton (Naval Research Lab)</b>	11:20 - 11:55 AM
Design of Materials through the Coupling of Length Scales	

<b>A. V. G. Chizmeshya (Arizona State Univ.)</b>	11:55 - 12:10 PM
Non-empirical Density Functional Description of the Thermoelastic Properties of Complex Ceramics	

<b>Dieter Wolf (Argonne)</b>	12:10 - 12:25 PM
Molecular-dynamics Simulation of Grain-boundary Diffusion Creep	

<b>Jack Mecholsky (Univ. of Florida)</b>	12:25 - 12:40 PM
Wear and Degradation of Hybrid Bearings: Experiments and Modeling	

<b>LUNCH &amp; ADJOURNMENT</b>	12:40 PM
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**NSF PROGRAMS ON COMPUTER AIDED DESIGN OF HIGH TEMPERATURE  
MATERIALS**

**Bruce G. Taggart**  
National Science Foundation

## CREEP DEFORMATION OF SILICON NITRIDE

**S. M. Wiederhorn and W. E. Luecke**  
National Institute of Standards and Technology  
Gaithersburg, MD 20899

Most commercial grades of silicon nitride exhibit a very high dependence of creep rate on stress. Although creep data can be fitted to the usual power-law functions, data often show curvature and systematic variations of slope with temperature and stress. In this paper, we present a new approach to the creep of ceramics like silicon nitride that are vitreous bonded. A review of experimental data suggests that in these materials creep is controlled by the rate of formation and growth of cavities. The critical step for deformation is shown to be the flow of the vitreous bonding phase away from the cavitation site. The parameters that determine the creep rate are the effective viscosity of the silicate phase, and the number of cavities that are active at any moment. By assuming that the hydrostatic stress distribution between silicate pockets is normally distributed, it is possible to derive a creep equation that very closely matches the secondary creep rate of commercial grades of silicon nitride. The creep rate is predicted to depend on the viscosity and amount of silicate phase in the silicon nitride, but not on the size of the silicon nitride grains.

# **SIMULATIONS OF VARIABILITY IN HIGH TEMPERATURE MECHANICAL PROPERTIES EMANATING FROM STATISTICALLY DISTRIBUTED MICROSTRUCTURAL PARAMETERS OF CERAMICS**

**I. Beyerlein<sup>1</sup>, S. L. Phoenix<sup>2</sup>, R. Raj<sup>2</sup>**

<sup>2</sup>Department of Mechanical Engineering  
University of Colorado at Boulder  
Boulder, CO 80309-0427

and

<sup>1</sup>Department of Theoretical and Applied Mechanics  
Cornell University  
Ithaca, NY 14853

High temperature mechanical properties of ceramics, e.g., silicon nitride, are often determined by a combination of interfacial sliding, cavitation at grain junctions, and cavity growth. A glass phase at grain boundaries plays a dominant role in these kinetic processes. Simulations of these processes were carried out with random distributions of the microstructure parameters (grain size, grain aspect ratio, and viscosity and thickness of the glass phase). The simulations included a provision for influence functions that describe the *time dependent* redistributions of stresses and strains among neighboring cavities. The most remarkable result of the simulations is a large variability (up to factors of ten) in the creep rate and the time-to-fracture for different random choices of the microstructure (but with the same average statistics). These simulations help to explain experimental results in the literature which show a similar variability in the fracture life of silicon nitride of specimens, taken from the same batch, at a fixed tensile load and temperature. The simulations afford schemes for microstructure design that may help to reduce the stochastic variation in the creep fracture life of ceramics.

## GRAIN BOUNDARY CHEMISTRY AND CREEP RESISTANCE OF ALUMINA

**Martin P. Harmer, Helen M. Chan and Jeffrey M. Rickman**

Materials Research Center

Lehigh University

Bethlehem, PA 18015

A dramatic improvement in the creep resistance of alumina is obtained by the addition of oversized isovalent cation dopants such as yttrium (Y) and lanthanum (La). It has also been shown that this decrease in creep rate is primarily a solid solution effect, with enhanced creep resistance obtained at dopant concentrations below the solubility limit. Further intriguing studies have shown that even greater resistance can be achieved by selective co-doping with, for example, Zr and Nd. From this work it has been suggested that the observed reduction in creep rate results from an inhibition of grain boundary diffusion, consistent with both high resolution secondary ion mass spectroscopy (SIMS) and analytical electron microscopy (AEM) data which reveal a high propensity for dopant segregation. Given that the dopants may also alter grain boundary structure upon segregation, we have also studied the effect of Y on the distribution of grain boundary misorientations by using electron backscattered Kikuchi Diffraction (EBKD). Computer simulation methods are being employed which permit the determination of boundary segregation profiles and the effect of segregants on grain boundary diffusion.

This work was sponsored by the Air Force Office of Scientific Research.

# **POLYMORPHS OF ALUMINA PREDICTED BY FIRST PRINCIPLES: IMPLICATIONS FOR THE RUBY PRESSURE SCALE**

**Renata M. Wentzcovitch**

Department of Chemical Engineering and Materials Science  
University of Minnesota

Fully optimized quantum mechanical calculations indicate that corundum ( $\text{Al}_2\text{O}_3$ ) transforms to the as yet unobserved  $\text{Rh}_2\text{O}_3$  (II) structure at approximately 78 GPa, and further transforms to the (*Pbnm*) perovskite structure at 223 GPa. The predicted x-ray spectrum of the  $\text{Rh}_2\text{O}_3$  (II) structure bears similarities to that of corundum, suggesting substantial amounts of the phase could go undetected in high-pressure x-ray data. It is therefore possible that the ruby ( $\text{Cr}^{+3}$ -doped corundum) fluorescence pressure scale is sensitive to the thermal history of the ruby chips in a given experiment.

## STRUCTURE AND TRANSPORT IN LEVITATED MELTS

**D. L. Price, S. Ansell, J. E. Enderby and M.-L. Saboungi**  
Argonne National Laboratory, Argonne, IL 60439

**S. Krishnan**  
Containerless Research Inc., Evanston, IL

A novel levitation method has been developed for the study of containerless materials at high temperature. Samples are levitated in a conical nozzle and melted with a laser, achieving temperatures in the range of 2000 - 3000 K. Structural measurements are made with x-rays from a synchrotron source, while transport coefficients are measured with electrodeless techniques. Results will be given for aluminum oxide, yttrium oxide and silicon in the supercooled and normal liquid states.

This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences, under Contract W-31-109-ENG-38, and Small Business Innovative Research Grants, Phase I and Phase II.

# **CREEP DAMAGE PROCESSES IN STRUCTURAL CERAMICS: EXPERIMENTAL STUDIES AND THEIR IMPLICATIONS FOR COMPUTATIONAL MODELING**

**Richard A. Page**  
Southwest Research Institute  
San Antonio, TX 78238

Although cavity nucleation, growth and coalescence form the basis for most creep damage processes in ceramics, considerable variation in the details of the process exists. The precise mechanism by which creep damage accumulates and ultimately leads to failure depends on factors such as temperature, stress, and microstructure. The complexities involved in developing creep damage accumulation models that are suitable for accurate lifetime predictions are, thus, quite obvious.

Because of the inherent complexities and the lack of detailed experimental results, nearly every model developed to date has involved explicit assumptions regarding the nature and relative homogeneity of the nucleation sites, the density of nucleated cavities, the kinetics of cavity nucleation, the growth rates of cavities, the morphological development of cavities, and the stresses or stress fields that drive the damage process. Until recently, the shortcomings of available experimental techniques have made such assumptions unavoidable.

The application of a number of relatively new techniques has now begun to provide answers to a number of these critical questions. This paper provides an overview of our efforts in this area. The results of small-angle neutron scattering measurements of cavitation kinetics and stereoisaging measurements of the strain fields associated with creep cracks and of grain boundary sliding will be presented. The experimental results will be combined with damage models to identify important areas for future computer modeling.

## **HIGH-TEMPERATURE SILICON CARBIDE FIBERS**

**Michael D. Sacks**

University of Florida, Gainesville, FL 32611

Silicon carbide (SiC)-based fibers were prepared by dry spinning of organosilicon polymer solutions and subsequent heat treatment of the polymer fibers. The Si:C ratio was varied such that both nearly single-phase SiC fibers and two-phase SiC + C fibers were fabricated. As-prepared fibers had fine diameters ( $\sim 10\ \mu\text{m}$ ) and high tensile strengths ( $\sim 3\ \text{GPa}$ ). Fibers were characterized using a variety of techniques including scanning and transmission electron microscopy, X-ray diffraction, scanning auger microprobe, X-ray photoelectron spectroscopy, etc. Fiber tensile strengths and bend stress relaxation behavior were determined after heat treatments at temperatures up to  $\sim 1900^\circ\text{C}$ . Important factors which lead to the development of high-strength, thermally-stable fibers will be discussed.



# **INSIGHTS ON DEFORMATION MECHANISMS FROM ATOMISTIC MODELING OF STRUCTURAL INSTABILITY IN SOLIDS**

**C. S. Jayanthi<sup>1</sup>, M. Tang<sup>2</sup>, S. Y. Wu<sup>1</sup>, J. A. Cocks<sup>1</sup>, S. Yip<sup>3</sup>**

<sup>1</sup>Univ. of Louisville, <sup>2</sup>Lawrence Livermore National Laboratory, <sup>3</sup>MIT

Atomistic simulations can provide a wealth of insightful details at the microscopic level on defect formation and migration during the onset of structural instability. We describe a novel and simple method for performing such analysis based on the formulation of instantaneous (time-dependent) measures of interatomic bond stability which depend on both the spatial (local configuration) and dynamical (soft mode vibration) character of the phenomenon. Utility of this method is demonstrated through a molecular dynamics study of dilatation-induced decohesion of a beta-SiC lattice.

## **SiC: GROWTH, SINTERING AND THERMAL CONDUCTIVITY**

**P. C. Clapp, S-H Wang, and J. A. Rifkin**

Center for Materials Simulation  
Institute of Material Science  
Univ. of CT, Storrs, CT, 06269-3136

Using molecular dynamics simulation methods combined with Tersoff three body potentials for SiC, C and Si, studies have been made of vapor phase growth of SiC from a single crystal seed, the sintering processes among nanoparticles of SiC, and the thermal conductivity of SiC single crystal thin films with various defects present. Preliminary results will be presented and the vapor phase growth, as well as the sintering sequences, will be illustrated with computer movies.

# **DYNAMIC FRACTURE IN NANOPHASE CERAMICS AND DIAMOND FILMS: MULTIMILLION ATOM PARALLEL MOLECULAR-DYNAMICS SIMULATIONS**

**Andrey Omeltchenko, Kenji Tsuruta, Aiichiro Nakano,  
Rajiv K. Kalia, and Priya Vashishta**

Concurrent Computing Laboratory for Materials Simulations  
Department of Physics and Astronomy and Department of Computer Science  
Louisiana State University, Baton Rouge, LA 70803  
and

**Olga Shenderova and Donald W. Brenner**  
Department of Materials Science and Engineering,  
North Carolina State University, Raleigh, NC 27695-7907

A series of million-atom molecular dynamics simulations are performed on parallel computers to investigate fracture processes in nanophase silicon nitride and carbon-based materials. The simulations of carbon systems involve Brenner's reactive bond-order potential, which can adequately describe carbon in various bonding environments.

Molecular dynamics simulations are performed to investigate fracture processes in nanophase and crystalline silicon nitride. Mechanisms of energy dissipation are identified which result in improved mechanical properties of the nanophase system.

Simulations of dynamic fracture in a graphite sheet are carried out to investigate dynamics of crack propagation and self-affine properties of fracture surfaces. Results for the local-stress distribution and the branching instability at the crack tip will also be presented.

Hypervelocity impact of a diamond crystallite on a diamond film is studied as a function of the velocity of the crystallite. At a velocity of 8 km/s the crystallite goes deep into the film but then rebounds and remains virtually intact. Following the impact local graphitization is observed in the diamond film. At higher velocities crater formation is observed and the cluster disintegrates completely.

Fracture in diamond films is studied for different crystallographic orientations. The effects of grain boundaries and packing faults on the crack propagation are also investigated.

This work was supported by DOE (Grant No. DE-FG05-92ER45477), NSF (Grant No. DMR-9412965), AFOSR (Grant No. F 49620-94-1-0444), USC-LSU Multidisciplinary University Research Initiative (Grant No. F 49620-95-1-0452), Army Research Office (Grant No. DAAH04-96-1-0393), and Louisiana Education Quality Support Fund (LEQSF) (Grant No. LEQSF(96-99)-RD-A-10).

## SCALING PROPERTIES OF CRACKS

Elisabeth Bouchaud

O.N.E.R.A. (OM), 29 Avenue de la Division Leclerc  
B.P. 72, 92322 Châtillon Cedex, FRANCE

The fracture surfaces of various materials, analysed with different experimental techniques, have been shown to exhibit scaling geometrical properties in a certain range of length scales. Furthermore, the roughness index characterising these self-affine properties is in most cases close to the value 0.8, which was conjectured to be a *universal* critical exponent, i.e. independant of the fracture mode and of the material.

In order to understand this striking property, it has been suggested that the recent progresses made in statistical physics on the problem of line propagation through randomly distributed obstacles could be useful. In the problem of fracture, the moving line would be the fracture front, the morphology of which determines one of the fracture surfaces, which is just the *trace* it leaves behind it. Although these models are not yet really adapted to describe fracture, they have a few interesting predictions. When the external load is just sufficient for the front to free itself from the pinning microstructural obstacles, the crack velocity  $v$  tends to zero, and the models predict a fracture surface morphology characteristic of the vicinity of the so-called *depinning transition*. For finite  $v$ , locally, at small enough length scales - smaller than a crossover length  $\xi$  -, the line is pinned, and the roughness is the one expected for a zero velocity. At length scales larger than  $\xi$ , the expected morphology of the fracture surface is different.  $\xi$  decreases with  $v$  as a power law, and diverges when  $\xi$  tends to zero.

Our recent experiments investigate both the fatigue fracture surfaces of a metallic alloy, and the stress corrosion fracture surfaces of a silicate glass as a function of crack velocity. It is shown that in both cases, there are two fracture regimes, which have a well defined self-affine signature. At large enough length scales, the universal roughness index 0.8 is recovered. In the case of the metallic material, it could be measured over five decades of length scales (0.5nm-0.5mm). At smaller length scales, the roughness exponent is close to 0.5. The crossover length  $\xi$  separating these two regimes exhibits a power-law decrease with the measured crack velocity. This suggests that fracture of heterogeneous materials could be seen as a dynamic phase transition.

Contrarily to the critical exponents, the length scales characterising the morphology of these surfaces (self-affine correlation length, "spikiness", crossover length...) are strongly material dependant. The scaling domain may extend up to the millimeter size in the case of metallic alloys, to the centimeter for rocks, while it hardly exceeds a hundred nanometers for glass or ceramics. It is argued that, via the microstructure, they are strongly correlated to the fracture toughness.

## **EFFECT OF SMALL ALUMINUM ADDITIONS ON MECHANICAL, ELASTIC AND STRUCTURAL PROPERTIES OF MONOCRYSTALLINE C11b MoSi<sub>2</sub>**

**P. Peralta, F. Chu, S. A. Maloy, P. Santiago, J. J. Petrovic, and T. E. Mitchell**

Materials Science and Technology Division, MSK765  
Los Alamos National Laboratory, Los Alamos, NM 87545

The Vickers hardness of monocrystalline C11b MoSi<sub>1.943</sub>Al<sub>0.057</sub> was measured at room temperature on the (001) and (110) planes for three different orientations of the indenter diagonal and compared to measurements performed in pure MoSi<sub>2</sub>. The presence of aluminum uniformly decreases the hardness and significantly changes the slip patterns around the indents, as compared to pure MoSi<sub>2</sub>. The elastic properties were obtained using Resonant Ultrasound Spectroscopy (RUS) and some anisotropic and effective moduli were found to be up to 10% lower than those of pure MoSi<sub>2</sub>. The lattice parameters were only slightly larger (less than 1%) than those of the pure material. The Peierls stresses were estimated for the known slip systems of MoSi<sub>2</sub> using the elastic and structural measurements for the Al alloyed crystal and the results correlated with the changes observed in the slip patterns.

# **A TOTAL ENERGY STUDY OF PHASE STABILITY AND MECHANICAL PROPERTIES OF LAVES PHASE COMPOUNDS**

**S. P. Chen, A. H. Ormeci, J. M. Wills, R. C. Albers, and O. Eriksson**

Theoretical Division  
Los Alamos National Laboratory  
Los Alamos, NM, 87545

First-principles electronic structure calculations based on a full-potential linear muffin-tin orbital method have been used to study the electronic and mechanical properties of the C15 and C14 Laves phase compounds,  $\text{NbCr}_2$  and  $\text{HfV}_2$ . The lower total energy structure for  $\text{NbCr}_2$  is found to be the C15 structure as opposed to the C14 structure for  $\text{HfV}_2$ . The calculated unit cell volume, elastic moduli, cohesive energies and heats of formation will be compared with experiments.

**THE APPLIED AND COMPUTATIONAL MATHEMATICS PROGRAM AT DARPA**

**Anna Tsao**  
DARPA

# NEARLY SINGULAR FIELDS: ELECTROSTATICS AND ELASTOSTATICS OF COMPOSITE MATERIALS

**Leslie Greengard**

Courant Institute, NYU, 251 Mercer Street, New York, NY 10012

An important area of research in materials science concerns the determination of the effective transport and mechanical properties of composites. There are a variety of theoretical approaches to this problem, including the derivation of rigorous bounds, effective medium theory, asymptotic approximations, Monte Carlo simulations, and direct solution of the governing equation. One advantage of the direct solution approach is that the desired properties are obtained with arbitrary precision, controlled only by the accuracy of the numerical method. A second advantage is that, having access to pointwise features of the solution, it is possible to study local field fluctuations, flicker noise, and breakdown phenomena.

A variety of numerical methods can be used for direct solution of the field equation, including finite difference and finite element methods, but we will restrict our attention to methods based on potential theory. Two approaches will be described. The first is an adaptive, high-order accurate integral equation solver with a posteriori refinement, which is suitable for arbitrary geometries. The second is a special method of images designed to study random dispersions of disks. Both methods are accelerated using the fast multipole method, and are capable of handling thousands of inclusions even when they are closely spaced and give rise to nearly singular fields.



# **ENERGY-BASED MODEL OF COMPRESSIVE SPLITTING IN HETEROGENEOUS BRITTLE SOLIDS**

**K. Bhattacharya, M. Ortiz, and G. Ravichandran**

Applied Mechanics, 104-44

California Institute of Technology, Pasadena, CA 91125

Confined heterogeneous brittle solids loaded under far-field uniaxial compression are often observed to split along the loading axis. This talk will present a theory which accords this phenomenon an energetic interpretation: the solid splits because in so doing it reduces its total energy, defined as the sum of bulk strain energy and surface energy. The heterogeneous microstructure gives rise to a complex stress distribution in the intact solid. The change in energy due to the release of the microstructural stresses may exceed the cost in fracture energy. Critical conditions for splitting are formulated for polycrystalline solids as a function of readily measurable material properties and applied stresses. The predictions of the theory are found to be in remarkably good agreement with experimental observations in ceramics and rocks.

## MICROSCOPIC MISFIT STRAINS IN POLYCRYSTALS

**Oscar P. Bruno**

Applied Mathematics, 217-50

Caltech, 1200 E. California Blvd., Pasadena, CA 91125

I will present an approach to the solution of elasticity problems in polycrystals supporting microscopic misfit strains. This approach is applicable to polycrystals whose grains or intergrain boundaries undergo arbitrary misfit deformations, such as those associated with thermal expansion, martensitic transformations, etc., possibly including grain boundary fracture. I will also present mathematically rigorous upper bounds for the calculated energy values, demonstrating the accuracy of the numerical results. Our numerics are based on consideration of a large number of Eshelby-type solutions in the small crystallites and grain boundaries making up the polycrystal; the energy minimization problem is then solved by means of simulated annealing. Imposed boundary conditions interact with the misfits through the elasticity equations, and lead to a statistically correlated array of misfit strains. Explicit numerical results will be given for martensitic transformations in polycrystals; a corresponding study of thermal shock in polycrystalline ceramics is currently in progress.

## COARSENING OF EUTECTIC AND DISCONTINUOUS LAMELLAR MICROSTRUCTURES

**Alan J. Ardell**

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Directionally solidified metallic or ceramic alloys of near-eutectic composition are attractive materials for high-temperature structural applications. From a morphological perspective, most directionally solidified, two-component eutectics consist either of alternating plates (lamellae) of the two phases, or of rods or fibers of the minor phase embedded in a continuous matrix. Some eutectics, however, solidify with an interconnected maze-like microstructure that is sometimes referred to as "Chinese script". The elevated-temperature mechanical properties of these natural composite materials depend on a characteristic spacing of the minority phase (e. g. the interlamellar spacing), and are typically poorer as the spacing increases. The as-grown spacing is governed by the solidification conditions, but microstructures generally coarsen at high temperatures and eutectic microstructures are no exception. The coarsening of eutectic microstructures can occur by several different processes. Rod eutectics have been observed to coarsen by the two-dimensional equivalent of diffusion-controlled Ostwald ripening, but they also coarsen by the movement of paired microstructural faults called terminations and branches. Lamellar eutectics nearly always coarsen by the motion of terminations and branches, but discontinuous coarsening is another, totally different, mechanism that can adversely affect their microstructural stability. In this paper all the mechanisms of microstructural coarsening will be reviewed and examples of the different types of behavior will be presented. Most of the quantitative experiments to date have been done on metallic eutectics, but some of the (quite limited) data on ceramic systems will also be presented and discussed.

# COMPUTER SIMULATION OF MICROSTRUCTURE IN METAL AND CERAMIC SYSTEMS. NEAR OR REMOTE FUTURE

**A. G. Khachaturyan and S. Semenovskaya**

Department of Ceramics, Rutgers University

and

**Y. Wang**

Department of Materials Science and Engineering, Ohio State University

The strain-accommodating mechanism of formation of coherent microstructures in phase transformations is considered. Difficulties of the theory and the ways of their overcoming are discussed. It is shown that the developed Stochastic Kinetic Field non-linear integro-differential equation which take into account the morphology-dependent coherency strain is a proper vehicle to provide a realistic simulation of different types of transformations. A set of computational algorithms based on these equations allows us to realistically simulate the coherent microstructures and their evolution as well as to predict the effect of the processing parameters on this evolution. In the proposed approach, the input data are the macroscopic parameters of the system which are usually known (crystal lattice parameters, symmetry of phases, elastic moduli, phase diagram and interfacial energy). The initial condition is a homogeneous parent state "quenched" into a two-phase field. The output data are the sequence of the microstructure images, which are visualizations of numerical solution of the kinetic equation, the dynamics of their evolution, the temporal dependence of the thermodynamic and other macroscopic parameters of interest. Examples of the simulated microstructure evolution in decomposing alloys and ceramic systems and in the martensitic transformations are presented. Their comparison with the observation results shows excellent agreement. We believe that the simulation results demonstrate that advancing supercomputer environment will be able soon to support using realistic simulations for practical applications in a computer-assisted materials design and to support further improvements of the model. The research was supported by grants from Division of Materials Research of the NSF and Division of Materials Science of the DOE

# FINGERING INSTABILITY IN DISLOCATION ANNIHILATION

**Robin L. B. Selinger and Ming Li**

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We show that a screw dislocation under the attractive force of a nearby free surface can undergo a fingering instability, in which one or more of the line's vibrational modes become unstable. The resulting line profile takes on a characteristic sine wave shape as the lowest vibrational mode grows most rapidly. A linear stability analysis that approximates the dislocation as a damped elastic string indicates that the line undergoes a sequence of transitions as it approaches the free surface, changing first from underdamped to overdamped, then from overdamped to unstable when the lowest vibrational mode begins to grow. As the line approaches closer to the free surface, more and more vibrational modes become unstable, though the lowest mode dominates. We discuss the possible role of the instability in the evolution of dislocation microstructure in bulk materials and in thin films. Simulation data are presented with emphasis on the role of elevated temperature.

# COMPARISON OF PHASE-FIELD AND SPIN MODELS FOR COARSENING PROCESSES

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and

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Discrete, mesoscale models including the phase-field model and spin model have recently been used to examine many microstructural evolution processes. The phase-field approach represents microstructure using continuum fields mapped on a discrete lattice, resulting in diffuse internal interfaces. The evolution of field variables occurs via time-dependent Ginzburg-Landau equations. In spin models, discrete lattice points are assigned membership in a microstructural feature, so internal interfaces are sharp and faceted. Evolution occurs by a Monte Carlo energy minimization. Despite these differences, the two models give similar results. We will compare results from the two models for 2-D, isotropic grain growth and Ostwald ripening. Grain size distributions and moments are similar in both cases. In grain growth, topology and von Neumann relations are in good agreement. In Ostwald ripening, matrix fraction dependence of size distribution skewness follow similar trends. Appropriate application for each will be discussed.

This work performed at Sandia National Laboratories, supported by the U.S. Department of Energy under contract number DE-AC04-95AL85000.

# CONTINUUM FIELD KINETIC MODEL AND SIMULATION OF PRECIPITATION OF L12 ORDERED INTERMETALLICS FROM FCC SOLID SOLUTION

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and

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A phenomenological field kinetic model of coherent precipitation of L12 ordered intermetallics from a disordered fcc solid solution will be presented. It explicitly takes into account both, the lattice misfit strain and the four types of antiphase domains formed as a result of the L12 ordering. Based on the concentration wave representation of the L12 ordering, a coarse-grained free energy functional of concentration and long-range order parameters has been formulated. Its relation to the atomistic model will be discussed. Precipitation kinetics and microstructural development of gamma prime phase in Ni-based superalloys have been investigated by computer simulations based on this model. The results reveal new features which are attributed to the L12 ordering. The ordered nature of the precipitates changes the coarsening mechanisms and kinetics and greatly affects the morphology of the mesoscopic microstructure.

## DIRECTIONAL SOLIDIFICATION OF EUTECTIC CERAMICS

Ali Sayir

NASA Lewis Research Center

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The eutectic architecture, a continuous reinforcing phase within a higher volume phase or matrix, can be described as a naturally occurring in-situ composite. The phases comprising a eutectic are thermodynamically compatible at higher homologous temperatures than man-made composites and as such offer the potential for superior high temperature properties and stability.

The mechanical properties of two phase eutectics can be superior to that of either constituent alone due to the strong constraining effects of the interlocking microstructure. The time dependent characteristics of directionally solidified  $\text{Al}_2\text{O}_3/\text{YAG}$  and  $\text{Al}_2\text{O}_3/\text{ZrO}_2(\text{Y}_2\text{O}_3)$  eutectics are presented. The relationships between lifetime, stress and temperature will be discussed. The solidification characteristics of  $\text{Al}_2\text{O}_3/\text{Y}_3\text{Al}_5\text{O}_{12}$  off-eutectic liquid and its relation to achieve in-situ composites materials will be treated at some length. Effects of composition on morphology and on crystallographic orientation are currently topics of investigation in alumina two-phase systems. The effects of varying volume percent of the two constituents and of the addition of dopants have been examined. The need for computer-aided approaches to describe and predict high temperature materials processing and properties will be discussed from an experimentalist's point of view.



## MODELING MICROSTRUCTURAL EVOLUTION UNDER EXTERNALLY APPLIED STRESSES

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Many high-temperature materials contain coherent second-phase precipitates which usually belong to a number of crystallographically different orientation variants. The physical properties of a materials are mainly determined by the morphology, volume fraction, and distribution of precipitates. In a coherent two-phase mixture, the morphology of precipitates and their distributions depend primarily on the elastic interactions arising from its lattice mismatch with the matrix. Therefore, one efficient way to control a two-phase microstructure is by applying external stresses during aging. The coupling between coherent strain and applied stress makes the differently oriented variants grow selectively, resulting in anisotropic distribution of the precipitates, and thus anisotropic properties of the material. In this talk, a continuum-field model will be presented, which can be effectively applied to modeling the microstructural evolution under externally applied stresses. Several examples will be discussed.

## COMPUTER SIMULATION OF GRAIN GROWTH KINETICS WITH SOLUTE-DRAG USING PHASE FIELD MODEL

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The effects of solute-drag on the grain growth kinetics were studied in 2-D computer simulations by using a diffuse-interface field model. It is shown that, in the low velocity/low driving force regime, the velocity of a grain boundary motion departs from a linear relation with driving force (curvature) with solute-drag. The nonlinear relation comes from the dependence of grain boundary energy and width on the curvature. The growth exponent  $m$  of power growth law for a polycrystalline system is affected by the segregation of solutes to grain boundaries. With the solute-drag, the growth exponent  $m$  can take any value between 2 and 3 depending on the ratio of lattice diffusion to grain boundary mobility. The grain size and topological distributions are unaffected by solute-drag, which are the same as those in a pure system.

## THE INTERFACE BETWEEN MONAZITES AND HIGH TEMPERATURE CERAMICS

**Peter E. D. Morgan, David B. Marshall, Janet B. Davis, and Robert M. Housley**

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In several publications\* we have shown that the interface between monazites (more specifically  $\text{LaPO}_4$ ) and conventional ceramic materials: alumina, mullite, zirconias and others, are weak and easily debond under stress. This leads to several interesting and practical results. It engenders sliding/pull-out when alumina or mullite type fibers are coated with monazite in a ceramic matrix composite (CMC) making them notch insensitive with much distributed damage and with "plastic-like" stress-strain curves. Weak interfaces also lead to "machinable" diphasic ceramics containing the monazite - indeed, monazite itself appears to be machinable, and other mechanisms also appear to be involved.

Some qualitative suggestions as to why these interfaces are weak have been advanced\* based upon classical bonding ideas but the details, which should be very informative, appear to beg the application of calculational methods.

The discovery was somewhat counterintuitive as many phosphates are used as strong binders in ceramics.

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\* P. E. D. Morgan and D. B. Marshall, "*Ceramic Composites of Monazite and Alumina*", J. Am. Ceram. Soc., **78** 1553-63 (1995)

P. E. D. Morgan, D. B. Marshall and R. M. Housley, "*High Temperature Stability of Monazite-Alumina Composites*", J. Mat. Sci. Eng., **A195** 215-22 (1995)

D. B. Marshall, P. E. D. Morgan and R. M. Housley, "*Particulate composite of Mullite-Alumina*", J. Am. Ceram. Soc. (in preparation).

D. B. Marshall, P. E. D. Morgan, R. M. Housley and J. T. Cheung, "*High Temperature Stability of the  $\text{Al}_2\text{O}_3$ - $\text{LaPO}_4$  system*", J. Am. Ceram. Soc. (in press).

J. B. Davis, D. B. Marshall, P. E. D. Morgan and R. M. Housley, "*Machinable Ceramics Based on Rare-Earth Phosphates*", J. Am. Ceram. Soc. (in preparation).

## UNIVERSAL BEHAVIOR IN ADHESION OF SOME HIGH TEMPERATURE MATERIALS

**John R. Smith<sup>1</sup>, J. E. Raynolds<sup>2</sup>, E. R. Roddick<sup>2</sup>, and D. J. Srolovitz<sup>2</sup>**

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Processing and design of materials often involves issues of adhesion. The nature of the strong bonds which can form between materials in intimate contact is therefore of considerable interest. Because of the variety of materials found in these interfaces (metals, ceramics, intermetallics, and impurities), adhesion computations must be first-principles, self-consistent quantum-mechanical calculations. A number of years ago, the first such computations revealed an unexpected universality. It was found that the total energy versus interfacial spacing for a number of different metal contacts could be simply scaled onto a single curve. Subsequently it was found that this universality extended to a variety of materials in cohesion, chemisorption, and to diatomic molecules. More recently, it was shown that the universal behavior extends to Mo/MoSi<sub>2</sub> adhesion with and without monolayers of C, O, B, S, and Nb interfacial impurities. Impurity effects were found to be large and strongly dependent on impurity atom type. For example, S lowered the adhesive energy by approximately a factor of two. For the ceramic/metal interfaces MgO/Ag and MgO/Al with and without C and S impurities, universal behavior was again observed as were substantial impurity effects. For Al<sub>2</sub>O<sub>3</sub>/Cu, surface relaxation effects were found to be substantial, lowering the work of adhesion by a factor of three. The bimetallic interface NiAl/Cr accurately exhibited universal behavior, as expected. In all these cases electron density distributions help to illustrate the nature of the bonding, which varies from pure metallic to partially ionic - partially covalent.

## STRUCTURAL CORRELATIONS AND STRESS DISTRIBUTIONS AT SILICON/SILICON NITRIDE INTERFACE

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Using molecular dynamics (MD) simulations on parallel computers the interface structure, stress distributions, crack propagation and fracture in a  $\text{Si}_3\text{N}_4$  film on a crystalline Si(111) substrate are studied. The  $\text{Si}_3\text{N}_4$  system is described by two-body and three-body interactions accounting for charge transfer, polarizability and covalent effects; the silicon system interacts via the Stillinger-Weber potential. To model the interface, information about charge transfer is taken from LCAO electronic structure calculations [1]. MD data for structural correlations in the interfacial region and stress distribution in a Si/Si/  $\text{Si}_3\text{N}_4$  mesa will be presented. Results for crack propagation and fracture will also be discussed.

[1] G.-L. Zhao and M. E. Bachlechner, *Europhys. Lett.* **37**, 287 (1997)

This work is supported by the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, AFOSR, DOE, NSF, ARO, USC-LSU MURI from DARPA, and LEQSF.

# **THE PROCESSING AND FUNCTIONALITY OF NITRIDE, OXIDE, AND PHOSPHATE CERAMICS CHARACTERIZED BY NEUTRON SCATTERING**

**C.-K. Loong**

Intense Pulsed Neutron Source

Argonne National Laboratory, Argonne, IL 60439

Neutrons probe the organization and interactions of the building blocks of materials. The formation of atomic bonds and assemblage of networking molecules, crystalline grains, polymeric units, solute/solvent species, etc. over the length scale of 0.1-500 nm can be studied experimentally often under extreme conditions such as at high temperatures or under corrosive environment. Neutron-scattering data in terms of various particle-particle correlation functions can afford a rigorous, quantitative comparison with results from large-scale computer simulations. We first present an overview of capabilities of neutrons in the characterization of high-temperature materials. The interplay of the microscopic structure and atomic dynamics with macroscopic properties such as mechanical strengths, interfacial stresses, and magnetic behavior is emphasized. Specific examples on silicon nitride ceramic alloys, rare-earth modified zirconia and alumina, and phosphate minerals of monazite/xenotime studied recently at the DOE user facility IPNS of Argonne will be given to illustrate the complementarity between neutrons and high-performance computations. Work performed at Argonne National Laboratory is supported by the U. S. DOE-BES under the contract No. W-31-109-ENG-38.

## NEUTRON SCATTERING CHARACTERIZATION OF MICROSTRUCTURE IN URANIUM SILICIDES, CERAMIC COMPOSITES AND Ni-BASED ALLOYS

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Intense Pulsed Neutron Source

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Neutron scattering has proven to be a valuable tool for studying the microstructural properties of technologically important materials. The exceptionally high penetration power of neutrons enables the investigation of bulk materials, while superior scattering contrasts observed in many materials provide unique access to important properties. Macroscopic performance of components under extreme conditions, which ultimately determines their viability for special applications, is often closely related to microstructural properties such as particle size, residual stress and phase stability. Neutron scattering experiments performed with samples exposed to realistic environmental conditions provide direct correlations between microscopic and macroscopic properties. Neutron irradiation of uranium silicide (a prospective reactor fuel), is used here as a prototypical example of in situ residual stress generation and evolution, accompanied by direct amorphization. Neutron diffraction studies at IPNS identified structural instabilities which contributed to material failure. Highly accurate measurements of residual strains in ceramic composites are used to validate computer models for stress variation with temperature and the effects of interfacial fiber coatings on residual stress. Coarsening and lattice mis-match of g'-type  $\text{Ni}_3(\text{Al},\text{Si})$  particles in Ni-based alloys, which strongly influence coherency strains in these materials, are also measured directly using neutron scattering.

Work performed at Argonne National Laboratory is supported by the U. S. DOE-BES under contract No. W-31-109-ENG-38.

## **FUNDAMENTAL STUDIES OF SURFACES AND INTERFACES AT HIGH TEMPERATURE VIA MICRODESIGNED INTERFACES**

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In the mid-1980's, a method for fabricating highly controlled internal defect structures in ceramics was developed. This method relies on a combination of photolithographic processing, ion beam etching, and solid-state diffusion bonding. The approach is quite flexible, and can therefore be applied to a wide range of materials and materials combinations. The presentation will describe and illustrate the processing of a wide range of internal defect/ flaw structures, and the use of such structures as the basis for model studies. Topics that have been investigated using such microdesigned interfacial structures include: the flow and burnout of binders in porous media, the Wulff shape of doped and undoped sapphire, surface diffusion in doped and undoped sapphire, high temperature crack healing in sapphire and glass-containing aluminas, the Rayleigh instability of high aspect ratio phases in doped and undoped sapphire, grain boundary migration in alumina, the nondestructive evaluation of microdesigned buried defects, and the diffusive growth of cracks during high-temperature mechanical testing. The ability to reproduce the geometry and crystallography of features in doped and undoped material has allowed the interplay between crystallographic effects, doping effects, and morphological evolution and stability to be probed.

Highlights from prior and on-going work will be used to illustrate the research approach and the unique research opportunities that the method creates, with emphasis given to the more recent developments and extensions of this technique. Specifically, by combining the lithography based methods with atomic force microscopy, a new experimental approach for characterizing the Wulff shape of undoped and doped sapphire has emerged. The effects of temperature and impurities on relative surface energies are now being examined, and links between morphological stability and dopant-induced surface stabilization are indicated. In parallel, the use of lithography to produce preperurbed pore channels has provided a powerful new method for investigating surface stability and surface diffusion in sapphire. New insights on the role of surface energy anisotropy are emerging. In particular, apparent changes in the surface diffusivity brought about by doping may in fact reflect the effect of the dopant on the surface energy anisotropy. Finally, in tandem with these studies of solid-vapor interfaces, solid-solid interfaces are also being investigated, with particular emphasis on the role that low level dopant additions and dopant valance gradients can play on microstructural evolution. Doping stimulated anisotropies in grain boundary properties may allow the formation of novel microstructures exhibiting desirable properties or property gradient.



# **BOND-ORDER POTENTIALS: BRIDGING THE ELECTRONIC-ATOMISTIC LENGTH SCALE GAP FOR HIGH TEMPERATURE COVALENT CERAMICS AND INTERMETALLICS**

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The directional nature of the covalent bond in high-temperature ceramics and intermetallics is correctly described by the semi-empirical Tight Binding (TB) model. In this talk we outline how this TB description of the electronic structure may be used to derive an explicit angularly-dependent interatomic potential. This so-called Bond-Order Potential (BOP) is a many-atom expansion that gives the energy of any given bond in terms of its local environment. We show that, although the first term in this BOP expansion is similar to the usual Tersoff form, it is unable in principle to differentiate between different structure types. This requires inclusion of further terms in the BOP expansion. This is illustrated by the development of a new analytic Bond-Order Potential for carbon.

## AB INITIO CALCULATIONS OF INTERFACES IN MATERIALS: GRAIN BOUNDARIES IN SiC AND SiC/Al INTERFACES

**Masanori Kohyama and John Hoekstra**

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Some of the most important properties of high-temperature materials are strongly influenced by internal interfaces such as grain boundaries. And it is necessary to form interfaces with metals or some compounds in their practical applications. Thus it is of much importance to understand such interfaces from the atomic and electronic level. Currently, by virtue of the development of the first-principles molecular dynamics method, it is possible to apply ab initio calculations based on the density-functional theory to such complex systems. In this paper, we present our recent ab initio calculations of grain boundaries in SiC and SiC/Al interfaces using conjugate-gradient techniques [1], coupled with optimized pseudopotentials [2]. For the {122}  $\sigma=9$  boundary in SiC, fourfold coordinated models of polar and non-polar interfaces have been examined. It has been shown that interfacial C-C and Si-Si wrong bonds have a significant effect, by generating peculiar bond lengths and bond charges and localized states. For the SiC(100)/Al interface, both the Si and C terminated interfaces have been examined. Each interface displayed very different features, such as atomic configurations, bonding characteristics, adhesive energies, electronic structure and Schottky-barrier heights. It is clear that this kind of calculations can provide valuable insight into the nature of grain boundaries in ceramics and metal-ceramic interfaces, and contribute greatly to the science and technology for the design of such interfaces.

- [1] M.Kohyama, Modelling Simul. Mater. Sci. Eng. **4** (1996) 397.
- [2] N.Troullier and J.L.Martins, Phys. Rev. B **43** (1991) 1993.

## STRUCTURE AND DYNAMICS OF CONSOLIDATION AND FRACTURE OF NANOPHASE CERAMICS VIA PARALLEL MOLECULAR DYNAMICS

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Multi-million atom molecular-dynamics (MD) simulations are performed to investigate consolidation dynamics, vibrational properties, and long-range structural correlations in nanophase ceramics ( $\text{Si}_3\text{N}_4$  and  $\text{SiO}_2$ ). In the consolidated nanocrystalline ceramics the structure and the density-of-states in interfacial regions are similar to bulk amorphous systems. An enhancement of the low-energy phonon mode in interfacial region leads to larger specific heat than that of the single crystal. In the MD results for the static structure factor we find large peaks at small  $q$  regions ( $\sim 0.1 \text{\AA}^{-1}$ ) which account for the intercluster structural correlations in the consolidated system. These results will be compared with neutron scattering experiments. The dynamics of crack propagation, internal stress fields, and the morphology of fracture surfaces are also examined as a function of temperature and strain rate.

This work is supported by AFOSR, DOE, NSF, ARO, USC-LSU MURI from DARPA, and LEQSF.

## INTERFACES IN OXIDE FIBER-OXIDE MATRIX CERAMIC COMPOSITES

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For fiber reinforced ceramic composites to perform appropriately, i.e., to exhibit high fracture toughness and large strains-to-failure, there must be weak bonding along the fiber-matrix interface. This weak bonding allows interfacial debonding to occur in the presence of the stress field created at the front of a propagating crack. This interfacial debonding causes crack deflection along the fiber and an effective blunting of the crack. In addition, the interfacial debonding allows frictional sliding to occur between the fiber and the matrix leading to high fracture toughness of the material. To create this weakly bonded interface, fiber coatings are most commonly applied. Recent advances have shown that some  $ABO_4$  compounds such as scheelite,  $CaWO_4$  (proposed by Babcock & Wilcox), and monazite,  $LaPO_4$  (proposed by Rockwell Science Center), exhibit weak bonding to the polycrystalline alumina and aluminosilicate fibers which are commercially available. Other  $ABO_4$  compounds such as  $ErTaO_4$  do not provide the required interfacial properties and the resulting composites are brittle. Similarities in the tungstate and tantalate compounds to that of the phosphate family of  $ABO_4$  compounds (which were the first class of these  $ABO_4$  compounds to demonstrate weak bonding) will be presented as justification for their initial selection as promising coating concepts. Mechanical property results of composites containing scheelite and  $ErTaO_4$  fiber coatings will be discussed. Scanning electron microscopy and transmission electron microscopy were utilized to further document the presence or absence of interfacial debonding in the composite systems which were fabricated and tested and to document chemical stability between the coatings and the fibers.

# HYBRID CLASSICAL AND QUANTUM MODELING OF DEFECTS, INTERFACES, AND SURFACES

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Northwestern University

Electronic structures associated with defects, interfaces, and surfaces play a critical role in structural, electrical, and transport properties of materials. Atomic-scale information on electron densities, wavefunctions, and spectroscopic properties is needed to understand nanometer and micron scale behavior; however, the requisite composition and geometrical data are typically lacking. We describe a hybrid approach which makes use of classical Molecular Dynamics (MD) and Monte Carlo (MC) simulations, coupled to Embedded Cluster Density Functional (ECDF) algorithms. In this scheme, parametrized interatomic potentials are used in MD/MC to relax the defect or interface structure, subject to constraints imposed by electron microscopy and other experimental data. ECDF calculations are carried out at equilibrium, metastable, near-equilibrium geometries, and along transition paths. Charge and bond-order analysis, along with calculated cohesive energies, are used to analyze local bonding structure, and to check and refine the input potentials. Electron energy loss and X-ray near edge absorption spectra are computed for comparison with spatially resolved experimental data. Examples will be given for impurities in metals, doped grain boundaries versus free surfaces in iron, the electroceramic  $\text{SrTiO}_3$ , and the structural ceramic  $\text{CaWO}_4$ .

Supported by DOE and NSF/DMR

# STRUCTURAL PROPERTIES OF $\text{SiO}_2$ UNDER PRESSURES: FIRST-PRINCIPLES CALCULATIONS AND DATABASE FOR SEVERAL CRYSTALLINE CONFIGURATIONS

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The properties of various phases of silica are of great interest to earth and material scientists. The need of accurate database to calibrate realistic and reliable interatomic force models by results of first-principles calculations has become increasingly important. Here I will present *ab-initio* electronic and structural properties of  $\alpha$ -quartz, coesite, and stishovite under various pressures. The local-density-functional-theory framework was employed, with a plane-wave basis, and the norm-conserving pseudopotentials. A local optimization technique will be presented to relax the internal and external degrees of freedom at each pressure. The transition pressures among these three phases of crystalline structures were calculated to be in good agreement with experimental values. Some possible novel phases of silica at higher pressures will also be presented.

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## STRUCTURAL CORRELATIONS IN AMORPHOUS $\text{SiO}_2$ AT HIGH PRESSURES

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Amorphous silica under various conditions of temperature and pressure are studied using the molecular dynamics simulation approach. The simulations are based on an effective interaction potential with a two-body interaction (consisting of steric repulsion, Coulomb and charge-dipole interactions), and a three-body covalent interaction which includes bond bending and bond stretching terms. A significant size dependence effect is observed in the First Sharp Diffraction Peak (FSDP) in the neutron static structure factor. The effect of pressure on bond angle distributions, rings statistics and its relation to FSDP is analyzed. A critical analysis of the changes in the FSDP for densities ranging from 2.0 to 3.2 g/cm<sup>3</sup> and temperatures varying from 0 to 1500K will be reported. With densification we observe that the height of the FSDP decreases proportionally to the decrease of the number of six-fold rings. A large scale simulation is also performed under negative pressure to investigate structural properties and mechanical failure in microporous silica.

# DEVELOPMENT OF A VARIATIONAL APW METHOD AND ITS APPLICATION TO THE ELECTRONIC PROPERTIES OF IONIC COMPOUNDS

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The augmented plane wave (APW) method based on the density-functional theory with the local-density approximation and the muffin-tin (MT) approximation is a well-established tool to calculate the electronic states in solids. However, the conventional computational scheme encounters difficulties in approaching materials where anisotropic effects due to the lattice symmetry play an important role in determining the electronic structures and/or where multi-species of atoms are involved. The Kohn-Sham potentials are usually assumed to be spherically symmetric inside the MT spheres and there is no definite prescription to set the MT radii.

We have recently reformulated the APW method according to the Hohenberg-Kohn variational principle in the density-functional theory. In the variational APW scheme proposed here, the size of the MT spheres is so determined as to minimize the ground-state energy of a system as well as the shape of the MT potentials. The lattice-induced anisotropic effects on the electronic states can also be taken into account by exactly calculating the Coulombic energy. It is thus expected that the present scheme overcomes those difficulties in the conventional scheme. It is actually demonstrated that the variational treatment of the MT radii significantly improves agreement with experimental results for the lattice constant, the cohesive energy and the band structure in the alkaline tellurides, especially in  $\text{Li}_2\text{Te}$ , the most asymmetric compound among them.



# BAND-THEORETICAL APPROACH TO THE SUPERIONIC CONDUCTIVITY OF SOLID ELECTROLYTES

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The objective of the present study is to shed light on the mechanism of the superionic conductivity of solid electrolytes through electronic structure calculations. Silver ions, the radius of which is relatively large, show particularly large diffusivity in the haloid and chalcogenide matrices. Although a number of molecular dynamics simulations have been successfully applied to such a fascinating phenomenon, they critically depend on empirical interatomic potentials in which the steric size of Ag ions is set remarkably smaller than the corresponding Pauling radius.

We study here tellurides such as  $\text{Ag}_2\text{Te}$ ,  $\text{Cu}_2\text{Te}$  and  $\text{M}_2\text{Te}$  ( $\text{M} = \text{Li}, \text{Na}, \text{K}$ );  $\text{Ag}_2\text{Te}$  in the  $\alpha$  phase is a typical superionic conductor. Fully self-consistent APW calculations have been carried out for those systems with the anti-fluorite structure, where the exchange-correlation effects of electrons were treated in the local density approximation. We show the present calculations accurately reproduce the electronic properties of  $\alpha\text{-Ag}_2\text{Te}$  with characteristics of the narrow gap semiconductor. We pay special attention to the difference in the closed-shell structures between the noble-metal ions (d-shell) and the alkali ions (sp-shell) embedded in the Te sublattice with the p band. Comparison of the results for  $\text{Ag}_2\text{Te}$  and  $\text{Cu}_2\text{Te}$  enables us to discuss possible effects of the p-d hybridization on the onset of the superionic conductivity. The activation energies for the ionic diffusion are also estimated in good agreement with the experiments.

## **RESEARCH CHALLENGES IN THE DEVELOPMENT OF CERAMIC COMPOSITES**

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Interest in ceramic composites is a consequence of their potential for dramatically improved damage tolerance as compared to monolithic ceramics while delivering similar high temperature properties. The remarkable toughening effect resulting from proper combination of three brittle phases in the form of fiber, coating and matrix is a consequence of a particular sequence in the development of damage. It is understood that there are both beneficial and detrimental ways for damage to develop; hence, successful design of composites requires the management of the progression of such damage. The situation is greatly complicated by the fact that the most productive uses of ceramic composites are dependent upon the development of fiber coatings that not only promote the desired interfacial failure, but satisfy the additional requirement of being oxidation resistant. Identification of suitable materials and their evaluation, development and incorporation into composites would be enhanced by more thorough understanding of the underlying principles. These and other issues related to the development of ceramic composites will be reviewed with the intention of providing an overview of outstanding challenges and identifying topics of interest for future research.

## COMPUTATIONAL MATERIAL SCIENCE AS A TOOL FOR ALLOY DEVELOPMENT: UNDERSTANDING THE INFLUENCE OF CHEMISTRY ON FLOW BEHAVIOR IN TiAl

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The transition metal intermetallic alloys, such as TiAl and NiAl, are an important class of structural materials due to their low density, high melting temperature and excellent strength retention at high temperature. Alloy designers optimize the structural properties of these materials by varying alloy composition, microstructure and the volume fraction of the existing phases. Traditionally, the role alloying additions play in the deformation of metals has been separated into extrinsic and intrinsic effects. Extrinsic effects are manifested through changes in transformation kinetics, microstructural evolution, and phases present; while the intrinsic effects are reflected principally in dislocation dynamics. While extrinsic effects tend to dominate metallurgical design and development of structural materials, these are presently only amenable to empirically-based modeling and simulation. Conversely, significant progress has been realized in modeling and simulation of intrinsic properties for these systems. The results of several computational studies of the intrinsic effects of alloy chemistry in single crystalline TiAl will be reviewed. First principles and atomistic methods have been used to study dislocation mobility and stability as a function of alloy composition in single crystal g-TiAl. Also, the influence of coherent lamellar interfaces on dislocation mobility has been studied in polysynthetically twinned (PST) TiAl. Such efforts serve to improve our understanding of the structure-properties relationships in the ordered aluminides. However, direct application of these tools as a guide for alloy development has not been realized. Some of the shortfalls of these methods will be reviewed and possible directions for further research will be discussed.

# QUANTUM MECHANICS, FRACTURE MECHANICS AND FRACTAL GEOMETRY APPLIED TO HIGH TEMPERATURE MATERIALS

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The process of fracture is not understood well. We present several different approaches in an unified manner to understand the formation of fracture topography beginning with atomic processes. Molecular Orbital (MO) theory is used to identify the basic bond re-orientation that occurs during the application of strain from external sources. Quantum mechanics is used to identify this fundamental step as a ring contraction and bond slip which results in increased free volume. Molecular dynamics (MD) is used to model the surface structure which results from the linking of these free volume regions during fracture. Applied fractography and fracture mechanics are quantitative analyses of fracture surface features which provide the connection between external loading and material response at the macroscopic scale. Fractal geometry relates all of these analyses. Previous work has shown that the fracture energy,  $g$ , is related to the fractal dimensional increment,  $D^*$ , and elastic modulus,  $E$ :  $g=0.5 E a_0 D^*$  where  $a_0$  is a characteristic materials constant related to the structure at the crack tip. Macroscopic and AFM measurements of the fractal dimension and  $a_0$  relate the MO and MD modeling to experimental results. The final detailed description of the fracture process as a self-similar propagation of structural fractal fracture units is a result of atomic and molecular scale modeling and macroscopic measurements united by fractal concepts.

## MULTISCALE MATERIALS MODELING AT LLNL: PLASTIC FLOW IN BCC METALS

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The new era of Science-Based Stockpile Stewardship (SBSS) at the DOE Defense Programs national laboratories presents both real opportunities and real challenges for solving important materials problems of national significance. The mechanical properties of metals is one specific area where vast improvements in understanding and modeling capabilities are needed to meet the scientific objectives of SBSS. Multi-length-scale or multiscale materials modeling represents a very promising approach to this challenge. At LLNL, a specific multiscale-modeling initiative has been put forth on the problem of plastic flow in bcc metals. This initiative not only addresses a problem of programmatic importance, but if successful, could provide a general paradigm for modeling the mechanical properties and response of materials. An integrated and coordinated theoretical and experimental research program is emerging at the electronic-, atomic-, micro-, meso-, and continuum length scales involving multi-disciplinary teams at LLNL, as well as a substantial number of academic collaborators. Representative theoretical work at the electronic-, atomic- and micro-scales will be presented. At the electronic and atomic scale, ab initio all-electron electronic-structure and interatomic-potential methods serve as the basis to calculate a wide range of fundamental mechanical deformation and defect properties of bcc metals, including elastic moduli, ideal shear strength, and the atomic structure and energetics of vacancies, dislocations, and grain boundaries. The main focus of this effort is on dislocation behavior in prototype metals such as Mo and Ta, where rigorous generalized pseudopotential theory (GPT) has been used to develop model-GPT (MGPT) multi-ion interatomic potentials suitable for realistic atomistic simulations. An important long-range goal of the atomistic work is to provide all necessary input information on dislocation motion and interactions to microscale theories and simulations. At the microscale, 3D dislocation-dynamics simulation methods are being developed to predict stress-strain relations, strain-hardening behavior, and microstructural evolution in single crystal bcc metals. An important long-range goal at this length scale is a complete description of single-crystal plasticity.

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## ADVANCED VISUALIZATION IN SUPPORT OF MATERIALS MODELING AND DESIGN

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We will discuss progress and challenges in developing systems to support the interactive simulation and visualization of 1-100 million atom systems. Because of the complexity, novelty, and scale of these systems, we believe that traditional molecular modeling and visualization techniques will be inadequate. We are therefore exploring the use of spatially immersive virtual reality environments (e.g., CAVes and ImmersaDesks) for molecular model building, interactive modeling, and visualization of molecular nanostructures. Spatial immersive display (SID) devices surround the user in real space with a 3D computer-generated visual and audio scene that is responsive to the user's point of view, orientation, and action. SIDs typically are based on multiple large-format stereo projection systems and can provide 3D views to multiple users. We believe that immersive technology is needed to improve the ability for nanosystems design teams to develop physical "3D intuition" for structure, mechanism, and synthesis pathways of large-scale molecular designs. We also believe that nanotechnology CAD environments need to be usable by multiple people simultaneously (ideally as part of a collaboratory or collaborative design environment) and that SIDs offer significant advantages relative to traditional displays or head-mounted displays for collaboratively designing and exploring engineered molecular structures.

We will report on the results of experiments comparing nonimmersive, partially immersive, and fully immersive display systems on common modeling and visualization tasks associated with the engineering, modeling, and design of nanostructures. In particular, we are studying single- and multiple-user "projection/pursuit" tasks, such as identifying the location of defects in complex molecular lattice, understanding the dynamics of molecule-molecule interactions, and determining optimal space filling molecular designs.

If time permits, we will also report on the role and effectiveness of including explicit collaboration support in the modeling and visualization software environment.

## MULTILEVEL ALGORITHMS FOR COMPUTATIONAL HIGH-TEMPERATURE MATERIALS RESEARCH

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Molecular dynamics (MD) is a powerful tool for understanding how atomistic processes are related to macroscopic phenomena involving high-temperature materials. Recent developments in parallel processing technology and multiresolution numerical algorithms have established large-scale MD simulations as a new research mode for studying macroscopic materials phenomena such as fracture. However, many important processes (such as sintering and sol-gel processes) are characterized by time scales that are many orders-of-magnitude larger than atomic time scales. The required large system size and long simulated time are beyond the scope of current simulation technologies. We have developed new multilevel algorithms and physical models encompassing multiple levels of abstraction: i) space-time multiresolution schemes; ii) hierarchical dynamics via a rigid-body/implicit-integration/normal-mode approach; iii) adaptive curvilinear-coordinate load balancing; iv) variable-valence MD based on electronegativity equalization; and v) multilevel preconditioned conjugate gradient method. Multimillion-atom MD simulations are performed on parallel computers to study mechanical properties of high-temperature materials such as  $\text{Si}_3\text{N}_4$ .

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## MODIFIED GAUSS POINTS METHODS AND ITS APPLICATION IN HTMS

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Numerical analysis of high-temperature materials (HTMs) is highly necessary because it is less expensive and can be easily controlled as compared to the experimental. To demonstrate the non-linear behavior of high-temperature materials numerically, self-consistent constitutive model is essential. Meanwhile, numerous elements (as many as half million) are needed in simulating microstructure analysis. However this will lead to not only the low efficiency of numerical analysis but also the floating of solution due to the errors of the huge amount of computation. Significant efforts are being expended on the above problems. In this paper, the Monte Carlo method is employed to simulate a realistic 3-D microstructures with random distribution of the grains and their boundaries. A self-consistent model is applied successfully. The procedure and problems in the formulation and modification of microstructure analysis are presented in detail. The modified Gauss point method is derived to ensure both efficiency and accuracy in numerical analysis. A satisfactory result in terms of failure mode is obtained by comparing results from numerical to experimental studies.



# **SIMULATING HIGH TEMPERATURE CERAMIC SENSORS ACROSS ALL LENGTH SCALES**

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and

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Electrical transport in ceramic materials depends critically on structural properties and heterogeneities like grain boundaries, pores, second phases and impurity segregation at surfaces and grain boundaries. At the same time the transport properties are of key importance in materials used for devices such as sensors. We propose an integrated computational approach which unites the structural and transport modeling of electronic ceramic materials across a wide range of length scales from microscopic through mesoscopic to macroscopic. The high temperature oxide-based ceramic sensor materials are taken as model systems. At the microscopic level, we study gas absorption and reaction processes at the surface of grains through Monte Carlo modeling together with calculations of the percolation conductivity of the granular oxide. At the mesoscopic level, the field kinetic modeling is employed to describe the detailed microstructure development during sintering, from which the electrical conductivity of the sintered samples can be calculated. For the first time, the conductivity of the sample is calculated concurrently as the microstructure evolves. Finally, coarse graining of the mesoscopic field kinetic simulation results leads to an integrated phenomenological model that describes the gas reactions and percolation conduction at the macroscopic level. The contrast between different proposed reaction mechanisms is clearly shown.

## ISSUES INVOLVING DUCTILITY, TOUGHNESS, AND STRUCTURAL STABILITIES IN INTERMETALLICS AND MULTILAYERED HIGH TEMPERATURE MATERIALS

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Issues involved in ductility, toughness and structural stabilities in intermetallics and multilayered materials are discussed by reference to three different studies. In each, the role of computational work will be outlined. The first topic involves ductility and toughness issues in two-phase intermetallic compounds based on TiAl. Specifically, the deformation behavior of the minority phase  $\text{Ti}_3\text{Al}$  is considered and this is shown to exert a significant influence on the behavior of the alloys. The second topic involves ductile/brittle behavior observed in a set of recently developed Nb aluminides (B2 crystal structure), with compositions given by Nb-15Al-xTi, with x=10, 25 and 40 (all compositions in atomic %). Some of these alloys are extremely brittle at room temperature when deformed in tension, depending on composition. Experimental observations concerning this behavior will be presented, and possible reasons to account for the ductile/brittle behavior will be put forward. The third topic involves a study of the structural stabilities of thin metallic multilayers. In this work, multilayers of alternating layers of Al and Ti have been produced, and as the scale of the multilayer is reduced it is found that the structure of the Ti layers will transform from hcp to fcc, and then revert back to hcp as the scale is further reduced, and accompanying this latter reversion, the structure of the Al layers also transforms from fcc to hcp. Two models have been developed to explain why these structural transitions occur, and the details of these will be presented.

## **LARGE SCALE PARALLEL MOLECULAR DYNAMICS SIMULATIONS OF DUCTILE FAILURE**

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Understanding the failure mechanisms in materials is crucial to the development of new materials with high strength and toughness. Cracks and dislocations are the two major defects determining these mechanical properties. With the advent of massively parallel computing platforms, molecular dynamics (MD) simulations of over 100 millions of atoms in 3D are now feasible. Since 1993 we have developed a 3D MD code, SPaSM, [(S)calable (Pa)rallel (S)hort range (M)olecular dynamics], designed for very large scale simulations on a variety of parallel computing platforms. Using SPaSM over the past year we have performed massively parallel 3D molecular dynamics simulations with up to 35 million atoms to investigate ductile failure, obtaining mechanistic information at the atomistic level inaccessible to experiment. We observe dislocation loops emitted from the crack front - the first time this has been seen in computer simulations. The sequence of dislocation emission events, essential for crack front and differs strikingly from anything previously conjectured. The MD simulations will be illustrated by videos.

# MULTISCALE MODELING METHOD FOR PREDICTING MECHANICAL PROPERTIES OF POLYCRYSTALLINE COVALENT CERAMICS FROM FIRST PRINCIPLES

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Predicting brittle fracture strengths of polycrystalline ceramics requires detailed knowledge of energetic stabilities and stress concentrations at grain boundaries and related defects. In principle, structures, energies and stresses at grain boundaries can be accurately calculated at the atomic scale using, for example, density functional methods. In practice, however, first-principles calculations can be prohibitively compute intensive, especially for systems having long-range stress fields that require many atoms. Alternatively, grain boundaries can be modeled at the atomic scale using analytic potentials. While important qualitative fracture behavior can be obtained for relatively large systems with this approach, results produced by analytic potentials vary widely in reliability. This limits their use for predicting quantitative values of properties such as fracture strengths.

A new multiscale modeling method for calculating energies from first principles for tilt grain boundaries in covalent ceramics over an entire range of misorientation angle will be discussed. The method combines results from density functional calculations on a few key structures with a mesoscopic-scale disclination structural units model. The central feature of our method is that these key structures can be chosen to minimize the number of atoms required to encompass the entire stress field. The method is demonstrated by calculating energies for  $\langle 001 \rangle$  tilt grain boundaries in diamond at 197 different tilt angles spanning the entire misorientation range strictly from first principles. Extensions of our model to the prediction of fracture strengths for strained materials and more complicated microstructures will be discussed.

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## **HIGH TEMPERATURE THERMAL PROPERTY PREDICTIONS FOR MgO, KCl AND ZnS**

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The interrelationship of thermodynamic properties was evaluated from nearly zero K to the melting temperature for several model materials. In agreement with our previous studies for NaCl and Cu, the product of thermal expansion, isothermal bulk modulus, and molar volume approaches a constant at high temperature and resembles a specific heat  $C_v$  curve. An n-term Einstein model well represent this product at low to moderate temperature and provides a reasonable extrapolation to high temperatures when data are unavailable. By linearly approximating the high temperature bulk modulus, this model can evaluate and predict a lower limit for thermal expansion. Analytical expression for thermal expansion of MgO, ZnS, KCl are provided from nearly zero K to close to the melting or phase transition point. Specific heat, lattice parameters, bulk modulus and molar volume are given for the entire temperature range.

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## TESTS OF SINTERING LAWS AT THE NANOSCALE

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We are using Molecular Dynamics techniques with Embedded Atom Method potentials to study sintering, surface diffusion and grain boundary mobility in nanoparticle arrays. Preliminary results of the sintering studies on multi-particle arrays several hundred degrees below the melting point of pure Cu show unexpectedly large contributions from plastic deformation processes, mechanical rotations and highly driven surface and grain boundary diffusion effects. These results strongly indicate that the standard sintering theory developed for micron scale powders (e. g. Ashby sintering diagrams) will have to be heavily revised, if not abandoned, before accurate predictions of nanoscale sintering kinetics will be possible. A detailed test of Herring's scaling law has also been performed and it is found to fail over the entire range of sintering sizes at the nanoscale. Reasons for this failure will be offered. Computer movies will be displayed to illustrate the dynamics of the competing sintering processes.

# ATOMIC AND MOLECULAR PROCESSES STUDIED BY FIRST-PRINCIPLES MOLECULAR DYNAMICS

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Computational Materials Science entered a new era when Car and Parrinello proposed the first-principles molecular dynamics method (FPMD) in 1985. The FPMD method has three important implications:

1. An efficient algorithm for the electronic structure calculation for large systems;
2. Structural optimization and search for reaction paths by using the atomic forces calculated from the first principles;
3. Dynamical simulations by using the atomic forces calculated from the first principles.

The FPMD method is particularly useful for the cases where the chemical bonds are formed and broken. It is generally difficult to simulate such processes with the empirical classical interatomic potentials. It is also possible in the FPMD method to include the temperature effects in the electronic states. Although such attempts have not yet been pursued intensively, their impact may be significant in the study of high-temperature materials.

We have been studying atomic and molecular processes for various systems by using the FPMD method. Among them, I will talk on a couple of topics, such as initial processes in the homoepitaxial crystal growth of Si on the Si(001) surface, initial oxidation processes of the Si(001) surface and the dynamical simulations of chemical reactions.

## DESIGN OF MATERIALS THROUGH THE COUPLING OF LENGTH SCALES

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The Holy Grail of Computational Materials Science is the ability to describe matter on all length and time scales. This talk will concentrate on the former - we will describe a methodology, already implemented on parallel machines, to couple length scales from the continuum (Finite Element description), to the atomistic (Molecular Dynamics) to the electronic structure (Tight Binding). Our application will be crack propagation in silicon which is the "test-bed" for our methodology. However, this technique may readily be extended to high temperature ceramics for examining many phenomena where it is important to describe everything from the macroscopic to the microscopic.



# NON-EMPIRICAL DENSITY FUNCTIONAL DESCRIPTION OF THE THERMOELASTIC PROPERTIES OF COMPLEX CERAMICS

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Among the most difficult properties to extract reliably from simulations of complex ceramics is the elastic/stiffness tensor, and in particular, its pressure and temperature dependence. Large units cells containing rare-earth and transition metal atoms often vitiate the application of ab initio methods to this problem, while simplified schemes based on empirical interaction potentials usually reproduce one physical property at the expense of betraying another. We describe an efficient but quantitative simulation approach to the calculation of thermoelastic properties that has been used extensively within our group as a counterpart to experimental investigations. The variational principle is used to determine the minimum Gibbs free energy of a crystal composed of compressible Kohn-Sham atoms/ions. Many-body effects emerge naturally from a coupling between the ionic and electronic degrees of freedom, and all salient properties, including a thermodynamically consistent finite-T phonon spectrum can be readily obtained. Elastic properties are computed from a long wavelength analysis of the finite temperature and pressure quasi-harmonic phonon spectrum. We demonstrate the methods' performance by calculating a wide range of thermal and mechanical properties of the layered perovskites  $\text{KCa}_2\text{Nb}_3\text{O}_{10}$ ,  $\text{RbCa}_2\text{Nb}_3\text{O}_{10}$  and those of a number of alumina phases.

## MOLECULAR-DYNAMICS SIMULATION OF GRAIN-BOUNDARY DIFFUSION CREEP

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Molecular-dynamics (MD) simulations are used, for the first time, to study grain-boundary diffusion creep of a model polycrystalline silicon microstructure. Our fully dense model microstructures, with a grain size of up to 7.5 nm, were grown by MD simulations of a melt into which small, randomly oriented crystalline seeds were inserted. In order to prevent grain growth and thus to enable steady-state diffusion creep to be observed on a time scale accessible to MD simulations (of typically  $10^{-9}$  s), our input microstructures were tailored to (i) have a uniform grain shape and a uniform grain size of nm dimensions and (ii) contain only high-energy grain boundaries which are known to exhibit rather fast, liquid-like self-diffusion. Our simulations reveal that under relatively high tensile stresses these microstructures, indeed, exhibit steady-state diffusion creep that is homogeneous (i.e., involving no grain sliding), with a strain rate that agrees quantitatively with that given by the Coble-creep formula.

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## WEAR AND DEGRADATION OF HYBRID BEARINGS: EXPERIMENTS AND MODELING

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High quality silicon nitride ceramics have excellent high temperature strength, low density and excellent wear resistance. The combination of these properties makes silicon nitride an attractive material for the rolling elements in (metal/ceramic) hybrid high speed air turbine bearings. Wear in bearing balls limits the lifetime of hybrid bearings. Although the mechanisms of wear in steel components have been well characterized, the wear in silicon nitride has not been substantially characterized. This paper describes  $\text{Si}_3\text{N}_4$  bearing ball wear as a microcrack initiation and propagation process due to contact fatigue stresses. Experimental results agree with a proposed fracture model and with finite element analyses. The roles of the elastic modulus of the metal raceway and lubrication environment on the overall mechanical behavior of the bearing will be discussed in terms of crack propagation and spallation. We will show how the interactive investigation using experimental results and computer simulations led to the determination of the most likely failure mechanisms.